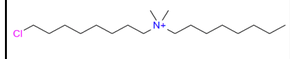
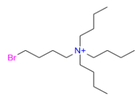
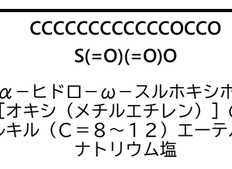
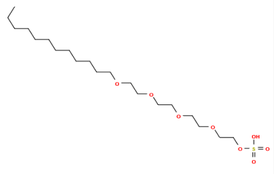
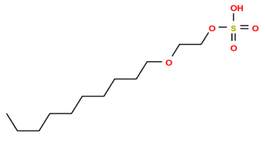
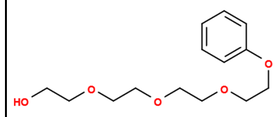
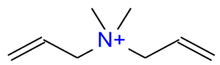
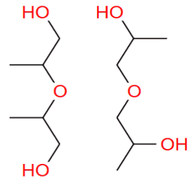
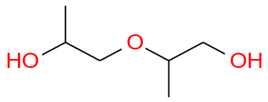
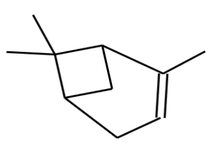
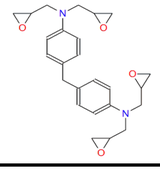
令和8年度 生態影響に関する優先度判定（一般化学物質）　今回新たに有害性クラスの付与を行う物質

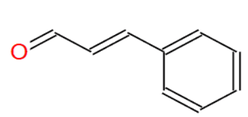
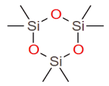
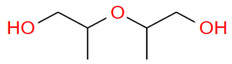
QSAR予測（KATE）

No	CAS RN®	SMILES・名称・構造式	log P (Estimated)	MW	QSAR Class	Type of Predicted Toxicity		Predicted Toxicity [mg/L]	Applicability Domain Judgement			Statistics of QSAR Regression			
						Organism	Acute or Chronic		Log P [Range]		structure	R^2	Q^2	RMSE	n
1	単位検討物質 （5538-94-3）	CCCCCCCCN(C)(C)CCCCCCCCCl N，Ｎ－ジメチル－Ｎ－オクチルオクタン－１－アミニウムの塩	2.95	305.97	CNOS_X halogen unreactive	Fish	Acute	20	in	[0.11, 5.81]	in	0.77	0.75	0.42	96(21)
					CNOS_X halogen unreactive	Daphnid	Acute	8.9	in	[0.78, 5.81]	out	0.86	0.85	0.39	46(10)
					CNOS_X halogen unreactive	Alga	Acute	14	in	[0.78, 5.10]	out	0.52	0.47	0.73	34(17)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.13	in	[-1.61, 5.99]	out	0.62	0.54	0.57	19(2)
					CNOS_X halogen unreactive	Alga	Chronic	3.2	in	[0.78, 5.81]	out	0.34	0.25	0.9	41(10)
					Unclassified Daphnid chronic	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	11(0)
2	1643-19-2	CCCCN(CCCC)(CCCC)CCCCBr テトラブチルアンモニウム＝ブロミド	2.05	322.37	CNOS_X halogen unreactive	Fish	Acute	92	in	[0.11, 5.81]	in	0.77	0.75	0.42	96(21)
					CNOS_X halogen unreactive	Daphnid	Acute	60	in	[0.78, 5.81]	in	0.86	0.85	0.39	46(10)
					CNOS_X halogen unreactive	Alga	Acute	76	in	[0.78, 5.10]	in	0.52	0.47	0.73	34(17)
					CNOS_X halogen unreactive	Alga	Chronic	11	in	[0.78, 5.81]	in	0.34	0.25	0.9	41(10)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.29	in	[-1.61, 5.99]	in(p)	0.62	0.54	0.57	19(2)
					Unclassified Daphnid chronic	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	11(0)
3(1)	2172642-87-2	CCCCCCCCCCCCCOCCO S(=O)(=O)O α－ヒドロ－ω－スルホキシポリ［オキシ（メチルエチレン）］のアルキル（Ｃ＝８～１２）エーテルのナトリウム塩 C12, 付加モル数：1	2.15	310.45	CNOS_X acid unreactive	Fish	Acute	360	in	[0.57, 5.00]	in	0.77	0.63	0.44	12(36)
					COS_X sulfonic acid	Daphnid	Acute	780	in	[0.48, 4.78]	in	0.98	-131.38	0.22	3(3)
					CNOS_X acid unreactive	Daphnid	Acute	120	in	[-0.80, 5.00]	in	0.34	0.14	0.72	16(23)
					CNOS_X acid unreactive sulfonic	Daphnid	Acute	120	in	[-0.80, 4.78]	in	0.58	-0.87	0.92	4(7)
					CNOS_X acid unreactive	Daphnid	Chronic	6.6	in	[-6.50, 5.98]	in	0.11	-0.44	0.86	22(11)
					CNOS_X acid unreactive sulfonic	Daphnid	Chronic	1.9	in	[-6.50, 5.95]	in	0.02	-2.07	0.68	7(3)
					CNOS_X acid unreactive sulfonic	Alga	Chronic	15	in	[-0.80, 5.95]	in	0.71	0.43	0.46	7(4)
					COS_X sulfonic acid	Fish	Acute	NA	NA	NA	NA	NA	NA	NA	1(5)
					CNOS_X acid unreactive sulfonic	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(10)
					Unclassified Fish chronic	Fish	Chronic	NA	NA	NA	NA	NA	NA	NA	0(0)
3(2)	2172642-87-2	CCCCCCCCCCCCCOCCOCCO CCOCCOS(=O)(=O)O C12, 付加モル数：4	1.32	442.61	CNOS_X acid unreactive	Fish	Acute	1600	in	[0.57, 5.00]	in	0.77	0.63	0.44	12(36)
					COS_X sulfonic acid	Daphnid	Acute	5100	in	[0.48, 4.78]	in	0.98	-131.38	0.22	3(3)
					CNOS_X acid unreactive	Daphnid	Acute	300	in	[-0.80, 5.00]	in	0.34	0.14	0.72	16(23)
					CNOS_X acid unreactive sulfonic	Daphnid	Acute	400	in	[-0.80, 4.78]	in	0.58	-0.87	0.92	4(7)
					CNOS_X acid unreactive	Daphnid	Chronic	11	in	[-6.50, 5.98]	in	0.11	-0.44	0.86	22(11)
					CNOS_X acid unreactive sulfonic	Daphnid	Chronic	2.9	in	[-6.50, 5.95]	in	0.02	-2.07	0.68	7(3)
					CNOS_X acid unreactive sulfonic	Alga	Chronic	35	in	[-0.80, 5.95]	in	0.71	0.43	0.46	7(4)
					COS_X sulfonic acid	Fish	Acute	NA	NA	NA	NA	NA	NA	NA	1(5)
					CNOS_X acid unreactive sulfonic	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(10)
					Unclassified Fish chronic	Fish	Chronic	NA	NA	NA	NA	NA	NA	NA	0(0)
3(3)	2172642-87-2	CCCCCCCCOCCOCCOCCO CCOS(=O)(=O)O C10, 付加モル数：1	-0.64	386.5	CNOS_X acid unreactive	Fish	Acute	23000	out(p)	[0.57, 5.00]	in	0.77	0.63	0.44	12(36)
					COS_X sulfonic acid	Daphnid	Acute	170000	out	[0.48, 4.78]	in	0.98	-131.38	0.22	3(3)
					CNOS_X acid unreactive	Daphnid	Acute	1000	in	[-0.80, 5.00]	in	0.34	0.14	0.72	16(23)
					CNOS_X acid unreactive sulfonic	Daphnid	Acute	2500	in	[-0.80, 4.78]	in	0.58	-0.87	0.92	4(7)
					CNOS_X acid unreactive	Daphnid	Chronic	16	in	[-6.50, 5.98]	in	0.11	-0.44	0.86	22(11)
					CNOS_X acid unreactive sulfonic	Daphnid	Chronic	2.8	in	[-6.50, 5.95]	in	0.02	-2.07	0.68	7(3)
					CNOS_X acid unreactive sulfonic	Alga	Chronic	100	in	[-0.80, 5.95]	in	0.71	0.43	0.46	7(4)
					COS_X sulfonic acid	Fish	Acute	NA	NA	NA	NA	NA	NA	NA	1(5)
					CNOS_X acid unreactive sulfonic	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(10)
					Unclassified Fish chronic	Fish	Chronic	NA	NA	NA	NA	NA	NA	NA	0(0)

No	CAS RN®	SMILES・名称・構造式	log P (Estimated)	MW	QSAR Class	Type of Predicted Toxicity		Predicted Toxicity [mg/L]	Applicability Domain Judgement			Statistics of QSAR Regression			
						Organism	Acute or Chronic		Log P [Range]		structure	R^2	Q^2	RMSE	n
3(4)	2172642-87-2	CCCCCCCCCCOCCOCCOCCOCCOS(=O)(=O)O C10，付加モル数：4	0.34	414.56	CNOS_X acid unreactive	Fish	Acute	6100	out(p)	[0.57, 5.00]	in	0.77	0.63	0.44	12(36)
					COS_X sulfonic acid	Daphnid	Acute	30000	out(p)	[0.48, 4.78]	in	0.98	-131.38	0.22	3(3)
					CNOS_X acid unreactive	Daphnid	Acute	550	in	[-0.80, 5.00]	in	0.34	0.14	0.72	16(23)
					CNOS_X acid unreactive sulfonic	Daphnid	Acute	1000	in	[-0.80, 4.78]	in	0.58	-0.87	0.92	4(7)
					CNOS_X acid unreactive	Daphnid	Chronic	13	in	[-6.50, 5.98]	in	0.11	-0.44	0.86	22(11)
					CNOS_X acid unreactive sulfonic	Daphnid	Chronic	2.8	in	[-6.50, 5.95]	in	0.02	-2.07	0.68	7(3)
					CNOS_X acid unreactive sulfonic	Alga	Chronic	59	in	[-0.80, 5.95]	in	0.71	0.43	0.46	7(4)
					COS_X sulfonic acid	Fish	Acute	NA	NA	NA	NA	NA	NA	NA	1(5)
					CNOS_X acid unreactive sulfonic	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(10)
					Unclassified Fish chronic	Fish	Chronic	NA	NA	NA	NA	NA	NA	NA	0(0)
3(5)	2172642-87-2	CCCCCCCCOCCOS(=O)(=O)O C8，付加モル数：1	0.18	254.34	CNOS_X acid unreactive sulfonic	Daphnid	Chronic	1.8	in	[-6.50, 5.95]	in	0.02	-2.07	0.68	7(3)
					CNOS_X acid unreactive sulfonic	Alga	Chronic	40	in	[-0.80, 5.95]	in	0.71	0.43	0.46	7(4)
					CNOS_X acid unreactive	Fish	Acute	4700	out(p)	[0.57, 5.00]	in	0.77	0.63	0.44	12(36)
					COS_X sulfonic acid	Daphnid	Acute	24000	out(p)	[0.48, 4.78]	in	0.98	-131.38	0.22	3(3)
					CNOS_X acid unreactive	Daphnid	Acute	380	in	[-0.80, 5.00]	in	0.34	0.14	0.72	16(23)
					CNOS_X acid unreactive sulfonic	Daphnid	Acute	720	in	[-0.80, 4.78]	in	0.58	-0.87	0.92	4(7)
					CNOS_X acid unreactive	Daphnid	Chronic	8.5	in	[-6.50, 5.98]	in	0.11	-0.44	0.86	22(11)
					CNOS_X acid unreactive sulfonic	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(10)
					Unclassified Fish chronic	Fish	Chronic	NA	NA	NA	NA	NA	NA	NA	0(0)
					COS_X sulfonic acid	Fish	Acute	NA	NA	NA	NA	NA	NA	NA	1(5)
3(6)	2172642-87-2	CCCCCCCCOCCOCCOCCOCCOS(=O)(=O)O C8，付加モル数：4	1.17	282.4	CNOS_X acid unreactive	Fish	Acute	1300	in	[0.57, 5.00]	in	0.77	0.63	0.44	12(36)
					COS_X sulfonic acid	Daphnid	Acute	4400	in	[0.48, 4.78]	in	0.98	-131.38	0.22	3(3)
					CNOS_X acid unreactive	Daphnid	Acute	210	in	[-0.80, 5.00]	in	0.34	0.14	0.72	16(23)
					CNOS_X acid unreactive sulfonic	Daphnid	Acute	300	in	[-0.80, 4.78]	in	0.58	-0.87	0.92	4(7)
					CNOS_X acid unreactive	Daphnid	Chronic	7.6	in	[-6.50, 5.98]	in	0.11	-0.44	0.86	22(11)
					CNOS_X acid unreactive sulfonic	Daphnid	Chronic	1.9	in	[-6.50, 5.95]	in	0.02	-2.07	0.68	7(3)
					CNOS_X acid unreactive sulfonic	Alga	Chronic	24	in	[-0.80, 5.95]	in	0.71	0.43	0.46	7(4)
					COS_X sulfonic acid	Fish	Acute	NA	NA	NA	NA	NA	NA	NA	1(5)
					CNOS_X acid unreactive sulfonic	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(10)
					Unclassified Fish chronic	Fish	Chronic	NA	NA	NA	NA	NA	NA	NA	0(0)
4(1)	単位検討物質 (9004-78-8)	c1ccccc1OCCO α－フェニル－ω－ヒドロキシポリ（オキシエタン－１，２－ジイル）（数平均分子量が1,000未満のものに限る。） 付加モル数：1 $C_8 H_{10} O_2$	1.1	138.16	CO_X primary alcohol	Fish	Acute	960	in	[-1.75, 5.26]	in	0.92	0.9	0.44	22(15)
					CO_X ether unreactive	Fish	Acute	690	in	[-1.75, 5.10]	in	0.87	0.86	0.52	44(17)
					CO_X alcohol unreactive w/ EO	Fish	Acute	500	in	[-1.75, 3.22]	in	0.98	0.97	0.19	5(6)
					CO_X primary alcohol	Daphnid	Acute	380	out(p)	[2.31, 5.26]	in	0.95	0.76	0.17	6(17)
					CO_X ether unreactive	Daphnid	Acute	600	out(p)	[1.34, 5.13]	in	0.75	0.69	0.59	19(19)
					CO_X primary alcohol	Alga	Acute	2300	out(p)	[2.31, 5.26]	in	0.91	0.79	0.36	6(16)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Acute	1100	out(p)	[1.34, 5.10]	in	0.68	0.58	0.6	12(17)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.28	in	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					CO_X ether unreactive	Daphnid	Chronic	10	in	[0.00, 4.66]	in	0.88	0.76	0.58	10(8)
					alcohol unreactive w/ EO alga	Alga	Chronic	17	in	[0.02, 3.22]	in	0.88	-1.81	0.34	4(3)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Chronic	29	in	[0.02, 5.13]	in	0.74	0.69	0.56	19(10)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Acute	NA	NA	NA	NA	NA	NA	NA	0(7)
					alcohol unreactive w/ EO alga	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(6)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	2(4)

No	CAS RN®	SMILES・名称・構造式	log P (Estimated)	MW	QSAR Class	Type of Predicted Toxicity		Predicted Toxicity [mg/L]	Applicability Domain Judgement			Statistics of QSAR Regression			
						Organism	Acute or Chronic		Log P [Range]		structure	R^2	Q^2	RMSE	n
4(2)	単位検討物質 (9004-78-8)	c1ccccc1OCCOCCOCCOCCO α－フェニル－ω－ヒドロキシポリ（オキシエタン－１，２－ジイル）（数平均分子量が1,000未満のものに限る。） 付加モル数：4 $C_{14}H_{22}O_5$ 	0.28	270.32	CO_X primary alcohol	Fish	Acute	9500	in	[-1.75, 5.26]	in	0.92	0.9	0.44	22(15)
					CO_X ether unreactive	Fish	Acute	6900	in	[-1.75, 5.10]	in	0.87	0.86	0.52	44(17)
					CO_X alcohol unreactive w/ EO	Fish	Acute	4700	in	[-1.75, 3.22]	in	0.98	0.97	0.19	5(6)
					CO_X primary alcohol	Daphnid	Acute	3600	out(p)	[2.31, 5.26]	in	0.95	0.76	0.17	6(17)
					CO_X ether unreactive	Daphnid	Acute	7100	out(p)	[1.34, 5.13]	in	0.75	0.69	0.59	19(19)
					CO_X primary alcohol	Alga	Acute	49000	out(p)	[2.31, 5.26]	in	0.91	0.79	0.36	6(16)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Acute	13000	out(p)	[1.34, 5.10]	in	0.68	0.58	0.6	12(17)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	1.1	in	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					CO_X ether unreactive	Daphnid	Chronic	160	in	[0.00, 4.66]	in	0.88	0.76	0.58	10(8)
					alcohol unreactive w/ EO alga	Alga	Chronic	130	in	[0.02, 3.22]	in	0.88	-1.81	0.34	4(3)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Chronic	190	in	[0.02, 5.13]	in	0.74	0.69	0.56	19(10)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Chronic	190	in	[0.02, 5.13]	in	0.74	0.69	0.56	19(10)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Acute	NA	NA	NA	NA	NA	NA	NA	0(7)
					alcohol unreactive w/ EO alga	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(6)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	2(4)
5	26062-79-3	C=CC[N+](C)(C)CC=C ポリ（ジアリルジメチルアンモニウムクロライド） 	-0.49	126.22	n+, N+	Fish	Acute	75	in	[-3.91, 5.18]	in	0.75	0.62	0.84	11(1)
					n+, N+	Daphnid	Acute	20	in	[-3.29, 5.18]	in	0.87	0.77	0.64	6(0)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.94	in	[-1.61, 5.99]	out	0.62	0.54	0.57	19(2)
					Unclassified Alga acute	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	18(13)
					Unclassified Daphnid chronic	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	11(0)
					Unclassified Alga chronic	Alga	Chronic	NA	NA	NA	NA	NA	NA	NA	17(2)
6	25265-71-8	CC(CO)OC(C)CO.CC(COCC(C)O)O ジプロピレングリコール 	-1.82	266.33	CO_X primary alcohol	Fish	Acute	580000	out	[-1.75, 5.26]	in	0.92	0.9	0.44	22(15)
					CO_X ether unreactive	Fish	Acute	430000	out	[-1.75, 5.10]	in	0.87	0.86	0.52	44(17)
					CO_X alcohol unreactive w/ EO	Fish	Acute	260000	out	[-1.75, 3.22]	in	0.98	0.97	0.19	5(6)
					CO_X primary alcohol	Daphnid	Acute	190000	out	[2.31, 5.26]	in	0.95	0.76	0.17	6(17)
					CO_X ether unreactive	Daphnid	Acute	680000	out	[1.34, 5.13]	in	0.75	0.69	0.59	19(19)
					CO_X primary alcohol	Alga	Acute	2.10E+07	out	[2.31, 5.26]	in	0.91	0.79	0.36	6(16)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Acute	1.10E+06	out	[1.34, 5.10]	in	0.68	0.58	0.6	12(17)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	5.9	out	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					CO_X ether unreactive	Daphnid	Chronic	31000	out	[0.00, 4.66]	in	0.88	0.76	0.58	10(8)
					alcohol unreactive w/ EO alga	Alga	Chronic	4300	out	[0.02, 3.22]	in	0.88	-1.81	0.34	4(3)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Chronic	4100	out	[0.02, 5.13]	in	0.74	0.69	0.56	19(10)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Acute	NA	NA	NA	NA	NA	NA	NA	0(7)
					alcohol unreactive w/ EO alga	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(6)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	2(4)

No	CAS RN®	SMILES・名称・構造式	log P (Estimated)	MW	QSAR Class	Type of Predicted Toxicity		Predicted Toxicity [mg/L]	Applicability Domain Judgement			Statistics of QSAR Regression			
						Organism	Acute or Chronic		Log P [Range]		structure	R^2	Q^2	RMSE	n
7	106-62-7	CC(CO)OCC(C)O ジプロピレングリコール 	-0.64	134.17	CO_X primary alcohol	Fish	Acute	29000	in	[-1.75, 5.26]	in	0.92	0.9	0.44	22(15)
					CO_X ether unreactive	Fish	Acute	21000	in	[-1.75, 5.10]	in	0.87	0.86	0.52	44(17)
					CO_X alcohol unreactive w/ EO	Fish	Acute	14000	in	[-1.75, 3.22]	in	0.98	0.97	0.19	5(6)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	1.1	in	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					CO_X primary alcohol	Daphnid	Acute	10000	out(p)	[2.31, 5.26]	in	0.95	0.76	0.17	6(17)
					CO_X ether unreactive	Daphnid	Acute	26000	out(p)	[1.34, 5.13]	in	0.75	0.69	0.59	19(19)
					CO_X primary alcohol	Alga	Acute	350000	out(p)	[2.31, 5.26]	in	0.91	0.79	0.36	6(16)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Acute	44000	out(p)	[1.34, 5.10]	in	0.68	0.58	0.6	12(17)
					CO_X ether unreactive	Daphnid	Chronic	800	out(p)	[0.00, 4.66]	in	0.88	0.76	0.58	10(8)
					alcohol unreactive w/ EO alga	Alga	Chronic	300	out(p)	[0.02, 3.22]	in	0.88	-1.81	0.34	4(3)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Chronic	370	out(p)	[0.02, 5.13]	in	0.74	0.69	0.56	19(10)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Acute	NA	NA	NA	NA	NA	NA	NA	0(7)
					alcohol unreactive w/ EO alga	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(6)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	2(4)
8	80-56-8	CC1=CCC2CC1C2(C)C 2，6，6－トリメチルビシクロ［3．1．1］ヘプター2－エン 	4.27	136.23	C_X hydrocarbon unreactive aliphatic w/o X	Fish	Acute	1.1	in	[2.58, 4.98]	in	0.73	0.68	0.36	21(4)
					narcotic group Fish Acute	Fish	Acute	1.3	in	[-0.63, 5.88]	in	0.87	0.87	0.43	152(33)
					C_X hydrocarbon unreactive aliphatic w/o X	Daphnid	Acute	0.48	in	[2.58, 5.74]	in	0.66	0.51	0.42	15(3)
					narcotic group Daphnid Acute	Daphnid	Acute	0.8	in	[1.08, 5.88]	in	0.72	0.71	0.42	81(24)
					narcotic group Alga Acute	Alga	Acute	0.84	in	[1.08, 5.26]	in	0.76	0.73	0.43	51(47)
					C_X hydrocarbon unreactive	Fish	Chronic	0.064	in	[1.52, 5.52]	in	0.78	0.68	0.43	11(0)
					Cnos_X unreactive Fish Chronic	Fish	Chronic	0.058	in	[1.52, 5.52]	in	0.76	0.68	0.43	12(0)
					narcotic group Fish Chronic	Fish	Chronic	0.06	in	[1.52, 5.81]	in	0.82	0.75	0.41	12(0)
					C_X hydrocarbon unreactive aliphatic w/o X	Daphnid	Chronic	0.16	in	[2.58, 5.74]	in	0.58	0.32	0.44	11(2)
					narcotic group Daphnid Chronic	Daphnid	Chronic	0.11	in	[-1.20, 5.88]	in	0.78	0.76	0.46	70(12)
					C_X hydrocarbon Alga Chronic	Alga	Chronic	0.35	in	[1.61, 5.52]	in	0.38	0.32	0.61	56(24)
					narcotic group Alga Chronic	Alga	Chronic	0.31	in	[0.69, 5.81]	in	0.57	0.53	0.69	58(28)
					C_X hydrocarbon unreactive aliphatic w/o X	Alga	Acute	0.43	out(p)	[2.58, 4.08]	in	0.66	0.38	0.47	6(10)
					C_X hydrocarbon unreactive aliphatic w/o X	Alga	Chronic	0.097	out(p)	[2.58, 4.20]	in	0.51	0.24	0.62	9(9)
9	28768-32-3	C1C(O1)CN(CC2CO2)C3 =CC=C(C=C3)CC4=CC =C(C=C4)N(CC5CO5)CC6CO6 	2.53	422.52	CNO_X amine sec,tert unreactive aliphatic	Fish	Acute	110	in	[-2.48, 4.67]	out	0.91	0.86	0.32	16(3)
					CNO_X amine sec,tert unreactive aliphatic	Daphnid	Acute	20	in	[-2.48, 4.67]	out	0.89	0.78	0.36	6(2)
					CNO_X amine sec,tert unreactive aliphatic	Alga	Acute	16	in	[-2.48, 3.87]	out	0.9	0.65	0.35	5(1)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.26	in	[-1.61, 5.99]	out	0.62	0.54	0.57	19(2)
					CNO_X amine sec,tert unreactive w/ N-Oxide,Nitroso	Daphnid	Chronic	1.4	in	[-0.80, 4.67]	out	0.81	0.74	0.49	15(2)
					CNO_X amine sec,tert unreactive aliphatic	Daphnid	Chronic	1.3	in	[-0.56, 4.67]	out	0.68	0.31	0.56	6(1)
					CNO_X amine sec,tert unreactive w/ N-Oxide,Nitroso	Alga	Chronic	1.2	in	[-2.48, 4.67]	out	0.7	0.63	0.84	22(2)
					CNO_X amine sec,tert unreactive aliphatic	Alga	Chronic	4.5	in	[-2.48, 3.87]	out	0.84	0.61	0.44	7(0)

No	CAS RN®	SMILES・名称・構造式	log P (Estimated)	MW	QSAR Class	Type of Predicted Toxicity		Predicted Toxicity [mg/L]	Applicability Domain Judgement			Statistics of QSAR Regression			
						Organism	Acute or Chronic		Log P [Range]		structure	R^2	Q^2	RMSE	n
10	104-55-2	C1=CC=C(C=C1)/C=C/C=O ３－フェニルアクリルアルデド 	1.82	132.16	aldehyde	Fish	Acute	6.9	in	[-1.40, 5.68]	in	0.23	0.16	0.7	52(0)
					CNO_X aldehyde normal aliphatic	Fish	Acute	9.5	in	[-1.40, 4.33]	in	0.63	0.39	0.34	12(0)
					aldehyde	Daphnid	Acute	6.1	in	[-1.40, 4.33]	in	0.54	0.4	0.52	15(1)
					aldehyde	Daphnid	Chronic	0.15	in	[-1.40, 4.33]	in	0.52	0.25	0.65	8(0)
					aldehyde	Alga	Chronic	0.63	in	[-1.40, 4.33]	in	0.28	-0.08	0.53	11(1)
					CNO_X aldehyde normal	Daphnid	Chronic	0.25	in	[-1.40, 4.33]	in(p)	0.7	0.28	0.59	5(0)
					CNO_X aldehyde normal	Daphnid	Acute	8.4	in	[-1.40, 4.33]	in(p)	0.64	0.4	0.5	10(1)
					CNO_X aldehyde normal	Alga	Chronic	0.94	in	[-1.40, 4.33]	in(p)	0.57	0.25	0.41	8(1)
					aldehyde	Alga	Acute	9.5	in	[-1.40, 3.35]	out	0.01	-0.5	0.65	10(2)
					CNO_X aldehyde normal	Alga	Acute	17	in	[-1.40, 3.35]	out	0.06	-0.67	0.55	7(2)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.15	in	[-1.61, 5.99]	out	0.62	0.54	0.57	19(2)
					CNO_X aldehyde, ketone	Fish	Acute	NA	NA	NA	NA	NA	NA	NA	2(0)
					CNO_X aldehyde, ketone	Daphnid	Acute	NA	NA	NA	NA	NA	NA	NA	1(0)
					CNO_X aldehyde, ketone	Alga	Chronic	NA	NA	NA	NA	NA	NA	NA	1(0)
11	541-05-9	C[Si]1(O[Si](O[Si](O1)(C)C)(C)C)C ２，２，４，４，６，６－ヘキサメチルシクロトリシロキサン 	5.64	222.46	Silicone atom	Fish	Acute	NA	NA	NA	NA	NA	NA	NA	0(1)
					Unclassified Daphnid acute	Daphnid	Acute	NA	NA	NA	NA	NA	NA	NA	10(4)
					Unclassified Alga acute	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	18(13)
					Unclassified Fish chronic	Fish	Chronic	NA	NA	NA	NA	NA	NA	NA	0(0)
					Unclassified Daphnid chronic	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	11(0)
					Unclassified Alga chronic	Alga	Chronic	NA	NA	NA	NA	NA	NA	NA	17(2)
12	108-61-2	CC(CO)OC(C)CO ２，２’－オキシビスプロパン－１－オール 	-0.64	134.17	CO_X primary alcohol	Fish	Acute	29000	in	[-1.75, 5.26]	in	0.92	0.9	0.44	22(15)
					CO_X ether unreactive	Fish	Acute	21000	in	[-1.75, 5.10]	in	0.87	0.86	0.52	44(17)
					CO_X alcohol unreactive w/ EO	Fish	Acute	14000	in	[-1.75, 3.22]	in	0.98	0.97	0.19	5(6)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	1.1	in	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					CO_X primary alcohol	Daphnid	Acute	10000	out(p)	[2.31, 5.26]	in	0.95	0.76	0.17	6(17)
					CO_X ether unreactive	Daphnid	Acute	26000	out(p)	[1.34, 5.13]	in	0.75	0.69	0.59	19(19)
					CO_X primary alcohol	Alga	Acute	350000	out(p)	[2.31, 5.26]	in	0.91	0.79	0.36	6(16)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Acute	44000	out(p)	[1.34, 5.10]	in	0.68	0.58	0.6	12(17)
					CO_X ether unreactive	Daphnid	Chronic	800	out(p)	[0.00, 4.66]	in	0.88	0.76	0.58	10(8)
					alcohol unreactive w/ EO alga	Alga	Chronic	300	out(p)	[0.02, 3.22]	in	0.88	-1.81	0.34	4(3)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Chronic	370	out(p)	[0.02, 5.13]	in	0.74	0.69	0.56	19(10)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Acute	NA	NA	NA	NA	NA	NA	NA	0(7)
					alcohol unreactive w/ EO alga	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(6)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	2(4)