

## Anticoagulants

TerraQSAR™ - LOGP computed octanol/water partition coefficients (CLOGPs).

For other toxicity and effect values, such as mammalian (rat/mouse) intravenous LD50, fish (fathead minnow) 96-hr LC50, estrogen receptor binding affinity (RBA), use TerraQSAR-RMIV, TerraQSAR-FHM, and TerraQSAR-E2-RBA programs, or consult TerraBase

SMILES	CAS	NAME	FORMULA	RTECS	MW	TerraQSAR-LOGP
[Na+].[O-]S(=O)(=O)C=C	25053-27-4	lyapolate sodium; sodium apolate [homopolymer; monomer structure shown]	C2H3NaO3S		130.10	-0.32
c1cc(Br)ccc1C2C(=O)c3ccccc3C2=O	1146-98-1	bromindione	C15H9BrO2	NK 5150000	301.14	2.90
c1cc(Cl)ccc1C2C(=O)c3ccccc3C2=O	1146-99-2	clorindione; Cumachlor	C15H9ClO2	NK 5250000	256.69	2.90
O=C2c1ccccc1C(=O)[C@]2([H])c3ccc(F)cc3	957-56-2	fluindione	C15H9FO2	NK 5700000	240.23	2.90
c1ccc2C(=O)C(c3ccccc3)C(=O)c2c1	83-12-5	phenindione; 2-phenylindane-1,3-dione	C15H10O2	NK 6125000	222.24	2.90
O=C(OCC)c1ccc(cc1)OC(=O)CCCCNC(N)=N	39492-01-8	gabexate	C16H23N3O4		321.38	2.61
c1ccccc1C(CC)C2=C(O)c3ccccc3OC2=O	435-97-2	phenprocoumon; 4-hydroxy-3-(1-phenylpropyl)-2H-1-benzopyran-2-one; AP-30	C18H16O3	GN 6769000	280.32	2.60
O=C1Oe2ccccc2C(O)=C1C(CC(=O)C)c3ccc(cc3)N(=O)=O	152-72-7	acenocoumarol	C19H15NO6	GN 4900000	353.33	2.60
c1ccc2C(O)=C(C(c3ccccc3)CC(=O)C)C(=O)Oc2c1	81-81-2	warfarin	C19H16O4	GN 4550000	308.33	2.60
N=C(N)C2=Cc1ccc(cc1C=C2)OC(=O)C3=CC=C(C=C3)NC(N)=N	81525-10-2	nafamostat	C19H17N5O2		347.38	0.54
O=C(OCCO)c1ccc(cc1)NC(=O)C=CC=CC=2OC(C)=O	62992-61-4	etersalate	C19H19NO6	DG 0929000	357.36	3.31
O=C2c1ccccc1C(=O)C2(CN3CCOCC3)C=4C=CC=CC=4	27591-42-0	oxazidione	C20H19NO3	NK 6020000	321.38	2.89
O=C2Oc1ccccc1C(O)=C2[C@]([H])(COC)C4=C(O)C=3C=CC=CC=3OC4=O	4366-18-1	coumetarol	C21H16O7		380.35	2.07
OC1=C(C(=O)O)c2ccccc12[C@@]([H])(CCC)c3ccc(cc3)CCCl	35838-63-2	clocoumarol	C21H21ClO3	DJ 2978500	356.85	2.60
c1ccccc1C[C@@H](NC)C(=O)N2CCC[C@H]2C(=O)N[C@H](C=O)CCNC(=N)N	105806-65-3	efegatran	C21H32N6O3		416.53	1.17
O[C@]([H])(C[C@]([H])(C2=C(O)c1ccccc1OC2=O)C3=C/C=C(/C)S3)C4=C/C=C/C(C)C=C4	22619-35-8	tiocloamarol	C22H16Cl2O4S		447.34	2.60
O=C(O)CN[C@@]([H])(C(=O)N1CC[C@]1([H])C(=O)NC/C2=C/C=C(C=C2)C(N)=N)[C@]3([H])CCCC3	159776-70-2	melagatran	C22H31N5O4		429.52	0.56
NC(=N)NCCC[C@]([H])([H])(NS(=O)=O)C2=CC=CC=C1C[C@@]([H])([H])CNC(=O)N3CC[C@]([H])([H])C(O)=O	74863-84-6	argatroban	C23H36N6O5S		508.64	-0.34
c1cc2onc(N)c2cc1n3nc(C(F)(F)F)cc3C(=O)Nc4ccc(cc4F)n5ccnc5CN(C)C	218298-21-6	razaxaban	C24H20F4N8O2		528.47	2.89
Oc1ccc(cc1)C[C@]([H])(NC(=O)c2ccc(cc2)C(N)=N)C(=O)N3CC[C@]([H])(C3)OCC(=O)O	144412-49-7	lamifiban	C24H28N4O6		468.51	1.20
O=C1CCCCN1c2ccc(cc2)N3C(=O)c4n(c5ccc(OC)cc5)nc(C(=O)N)c4CC3	503612-47-3	apixaban	C25H25N5O4		459.51	2.31



unavailable	9004-54-0	dextran	unavailable	HH 9230000	unavailable
unavailable	9005-49-6	heparin sodium	unavailable	MI 0700000	unavailable
unavailable [polymer]	9041-08-1	tinzaparin sodium; Reviparin sodium; sodium salt of depolymerized heparin; ardeparin sodium; several other CAS numbers; [a low-molecular-weight heparin]	unavailable	MI 0850000	unavailable
unavailable	9046-56-4	ancrod; proteinase obtained from the venom of the Malayan pit-viper Agkistrodon rhodostoma, acting specifically on fibrinogen	unavailable	UK 9575000	~ 35400

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