Bensulide

Other names:	Betasan
	Disan
	Disan (pesticide)
	N-(2-Mercaptoethyl)benzenesulfonamide S-(O,O-diisopropyl phosphorodithioate)
	N-[2-(O,O-Diisopropyldithiophosphoryl)ethyl]benzenesulfonamide
	O,O-Diisopropyl 2-(benzenesulfonamido)ethyl dithiophosphate
	O,O-Diisopropyl S-(2-benzenesulfonylaminoethyl) phosphorodithioate
	Phosphorodithioic acid, O,O-bis(1-methylethyl) S-[2-[(phenylsulfonyl)amino]ethyl] ester
	Phosphorodithioic acid, O,O-diisopropyl ester, S-ester with N-(2-mercaptoethyl)benzenesulfonamide
	Prefar
	R 4461
	S-«beta»-(Benzenesulfonamido)ethyl O,O-diisopropyl dithiophosphate
	S-Â«betaÂ»-(Benzenesulfonamido)ethyl O,O-diisopropyl dithiophosphate
	SAP
	SAP (herbicide)
Inchi:	InChI=1S/C14H24NO4PS3/c1-12(2)18-20(21,19-13(3)4)22-11-10-15-23(16,17)14-8-6-5-7
InchiKey:	RRNIZKPFKNDSRS-UHFFFAOYSA-N
Formula:	C14H24NO4PS3
SMILES:	CC(C)OP(=S)(OC(C)C)SCCNS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	397.51
CAS:	741-58-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Aqueous Solubility Prediction Method
log10ws	-4.20		Estimated Solubility Method
logp	3.773		Crippen Method
mcvol	287.330	ml/mol	McGowan Method
rinpol	2728.00		NIST Webbook
rinpol	2728.00		NIST Webbook
rinpol	2728.00		NIST Webbook
tf	307.55	K	Aqueous Solubility Prediction Method
tf	311.57 ± 0.20	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C741582&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point