Salithion

Other names:	4H-1,3,2-Benzodioxaphosphorin, 2-methoxy-, 2-sulfide
	Phosphorothioic acid, cyclic O,O-(methylene-o-phenylene) O-methyl ester
	Phosphorothioic acid, O-methyl ester, cyclic O,O-ester with o-hydroxybenzyl alcohol
	Saligenin cyclic methyl phosphorothionate
	4H-(1.3.2)Benzodioxaphosphorine, 2-methoxy-, 2-sulfide
	Dioxabenzofos
	K-9
	2-Methoxy-4H-1,2,3-benzodioxaphosphorine-2-sulfide
	Salithion-sumitomo
	2-Methoxy-4H-1,3,2-benzodioxaphosphorin-2-sulfide
	Dioxabenzophos
	Salition
	2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulphide
Inchi:	InChI=1S/C8H9O3PS/c1-9-12(13)10-6-7-4-2-3-5-8(7)11-12/h2-5H,6H2,1H3
InchiKey:	OUNSASXJZHBGAI-UHFFFAOYSA-N
Formula:	C8H9O3PS
SMILES:	COP1(=S)OCc2ccccc2O1
Mol. weight [g/mol]:	216.19
CAS:	3811-49-2

Physical Properties

Property code	Value	Unit	Source
log10ws	1.21		Crippen Method
logp	2.466		Crippen Method
mcvol	143.380	ml/mol	McGowan Method
rinpol	1609.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1672.00		NIST Webbook
ripol	2674.00		NIST Webbook
ripol	2674.00		NIST Webbook
tf	329.51 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	16.92	kJ/mol	327.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3811492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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