Propaphos

Inchi: InChI=1S/C13H21O4PS/c1-4-10-15-18(14,16-11-5-2)17-12-6-8-13(19-3)9-7-12/h6-9H,4-
InchiKey: PWYIUEFFPNVCMW-UHFFFAOYSA-N
Formula: C13H21O4PS
SMILES: CCCOP(=O)(OCCC)Oc1ccc(SC)cc1
Mol. weight [g/mol]: 304.34
CAS: 7292-16-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	4.749		Crippen Method
mcvol	230.560	ml/mol	McGowan Method
rinpol	2075.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2045.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2045.00		NIST Webbook
ripol	3021.00		NIST Webbook
ripol	3021.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7292162&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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