Propaphos sulfone

Inchi: InChI=1S/C13H21O6PS/c1-4-10-17-20(14,18-11-5-2)19-12-6-8-13(9-7-12)21(3,15)16/h6
InchiKey: OXMCGIWRESILLU-UHFFFAOYSA-N
Formula: C13H21O6PS
SMILES: CCCOP(=O)(OCCC)Oc1ccc(S(C)(=O)=O)cc1
Mol. weight [g/mol]: 336.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.82		Crippen Method
logp	3.430		Crippen Method
mcvol	242.300	ml/mol	McGowan Method
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R544675&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.