torac oxygen analog

Inchi: InChI=1S/C14H17ClNO5PS/c1-3-20-22(19,21-4-2)23-12(9-15)16-13(17)10-7-5-6-8-11(10
InchiKey: DGFSZLIRMFVRBS-UHFFFAOYSA-N
Formula: C14H17ClNO5PS
SMILES: CCOP(=O)(OCC)SC(CCl)N1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 377.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.00		Crippen Method
logp	3.762		Crippen Method
mcvol	253.280	ml/mol	McGowan Method
rinpol	2482.00		NIST Webbook
rinpol	2569.00		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=R490909&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.