Dimethoate oxygen analog

Inchi: InChI=1S/C5H12NO4PS/c1-6-5(7)4-12-11(8,9-2)10-3/h4H2,1-3H3,(H,6,7)
InchiKey: PZXOQEXFMJCDPG-UHFFFAOYSA-N
Formula: C5H12NO4PS
SMILES: CNC(=O)CSP(=O)(OC)OC
Mol. weight [g/mol]: 213.20

Physical Properties

Property code	Value	Unit	Source
hvap	73.65	kJ/mol	Cheméo Relay (1.0)
log10ws	0.27		Cheméo Relay (1.0)
logp	0.866		Crippen Method
mcvol	147.280	ml/mol	McGowan Method
tf	323.21	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1113026&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point