Demeton-O-OA

Other names:	demeton oxon
	Demeton-O, oxygen analog
Inchi:	InChI=1S/C8H19O4PS/c1-4-10-13(9,11-5-2)12-7-8-14-6-3/h4-8H2,1-3H3
InchiKey:	NMQDGOQOOUKIGM-UHFFFAOYSA-N
Formula:	C8H19O4PS
SMILES:	CCOP(=O)(OCC)OCCSCC
Mol. weight [g/mol]:	242.28

Physical Properties

Property code	Value	Unit	Source
hvap	74.86	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
log10ws	-0.55		Cheméo Relay (1.0)
logp	2.937		Crippen Method
mcvol	183.870	ml/mol	McGowan Method
rinpol	1550.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1550.00		NIST Webbook
tb	566.20	K	Cheméo Relay (1.0)
tf	205.98	K	Cheméo Relay (1.0)

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U289946&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point