Fensulfothion oxon sulfone

Other names:	O,O-Diethyl O-(p-methylsulfonyl)phenyl phosphate
	Phosphoric acid, diethyl 4-(methylsulfonyl)phenyl ester
	Fensulfothion oxon sulfone
	Diethyl 4-(methylsulfonyl)phenyl phosphate
	Dasanit O-analog sulfone
Inchi:	InChI=1S/C11H17O6PS/c1-4-15-18(12,16-5-2)17-10-6-8-11(9-7-10)19(3,13)14/h6-9H,4-5
InchiKey:	KUBUBYBFFRVFHD-UHFFFAOYSA-N
Formula:	C11H17O6PS
SMILES:	CCOP(=O)(OCC)Oc1ccc(S(C)(=O)=O)cc1
Mol. weight [g/mol]:	308.29

Physical Properties

Property code	Value	Unit	Source
hvap	108.14	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	Cheméo Relay (1.0)
log10ws	-2.29		Cheméo Relay (1.0)
logp	2.650		Crippen Method
mcvol	214.120	ml/mol	McGowan Method
tb	645.14	K	Cheméo Relay (1.0)
tf	341.55	K	Cheméo Relay (1.0)

Sources

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=C6132178&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point