Phosphinous acid, bis(trifluoromethyl) ester

Inchi: InChI=1S/C2HF6OP/c3-1(4,5)10(9)2(6,7)8/h9H
InchiKey: TUYWYUGWDOJWAE-UHFFFAOYSA-N
Formula: C2HF6OP
SMILES: OP(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 185.99
CAS: 359-65-9

Physical Properties

Property code	Value	Unit	Source
log10ws	0.92		Crippen Method
logp	2.415		Crippen Method
mcvol	75.990	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	46.60	kJ/mol	242.00	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=C359659&Units=SI

Legend

hsubt: Enthalpy of sublimation at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume