Methylphosphorochlorofluoridate

Other names: Methylphosphonyl chlorofluoride
Inchi: InChI=1S/CH3ClFOP/c1-5(2,3)4/h1H3
InchiKey: JJWNAEDAYJIUHA-UHFFFAOYSA-N
Formula: CH3ClFOP
SMILES: CP(=O)(F)Cl
Mol. weight [g/mol]: 116.46
CAS: 753-71-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	2.018		Crippen Method
mcvol	65.290	ml/mol	McGowan Method
sl	216.40	J/mol×K	NIST Webbook
tt	250.70 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	153.17	J/mol×K	298.15	NIST Webbook
hfust	11.85	kJ/mol	250.70	NIST Webbook
hfust	11.85	kJ/mol	250.70	NIST Webbook
sfust	47.28	J/mol×K	250.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C753719&Units=SI
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

Legend

cpl:	Liquid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tt:	Triple Point Temperature