Methylphosphonyldifluoride

Other names:	DF
	Methylphosphonic difluoride
	Phosphonic difluoride, methyl-
	Difluoro
	Difluoromethylphosphine oxide
	Methyl difluorophosphite
	Phosphonodifluoridic acid, methyl-
Inchi:	InChI=1S/CH3F2OP/c1-5(2,3)4/h1H3
InchiKey:	PQIOSYKVBBWRRI-UHFFFAOYSA-N
Formula:	CH3F2OP
SMILES:	CP(=O)(F)F
Mol. weight [g/mol]:	100.00
CAS:	676-99-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	1.748		Crippen Method
mcvol	54.820	ml/mol	McGowan Method
sl	208.34	J/mol×K	NIST Webbook
tt	236.34 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	145.14	J/mol×K	298.15	NIST Webbook
hfust	11.88	kJ/mol	236.34	NIST Webbook
hfust	11.88	kJ/mol	236.30	NIST Webbook
hfust	11.88	kJ/mol	236.30	NIST Webbook
sfust	50.26	J/mol×K	236.34	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C676993&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