Phosphonic acid, dimethyl ester

Other names:	Dimethyl phosphonate
	Dimethyl phosphite
Inchi:	InChI=1S/C2H7O3P/c1-4-6(3)5-2/h6H,1-2H3
InchiKey:	HZCDANOFLILNSA-UHFFFAOYSA-N
Formula:	C2H7O3P
SMILES:	CO[PH](=O)OC
Mol. weight [g/mol]:	110.05
CAS:	868-85-9

Physical Properties

Property code	Value	Unit	Source
affp	894.80	kJ/mol	NIST Webbook
basg	862.40	kJ/mol	NIST Webbook
hvap	46.70	kJ/mol	NIST Webbook
ie	10.53	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
ie	10.53	eV	NIST Webbook
log10ws	-1.30		Crippen Method
logp	0.669		Crippen Method
mcvol	77.110	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	46.70	kJ/mol	398.00	NIST Webbook
hvapt	48.30	kJ/mol	343.00	NIST Webbook
hvapt	47.90	kJ/mol	343.00	NIST Webbook
hvapt	46.40	kJ/mol	343.00	NIST Webbook
hvapt	46.00	kJ/mol	343.00	NIST Webbook
hvapt	45.40	kJ/mol	343.00	NIST Webbook
hvapt	38.70	kJ/mol	401.00	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=C868859&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:
https://www.chemeo.com/cid/38-164-8/Phosphonic-acid-dimethyl-ester.pdf
Generated by Cheméo on 2024-04-19 02:07:42.316898765 +0000 UTC m=+15781711.237476081.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.