

Phosphonic acid, dipropyl ester

Other names:	dipropyl phosphonate
Inchi:	InChI=1S/C6H15O3P/c1-3-5-8-10(7)9-6-4-2/h10H,3-6H2,1-2H3
InchiKey:	PVBGKAMVCZUNFQ-UHFFFAOYSA-N
Formula:	C6H15O3P
SMILES:	CCCO[PH](=O)OCCC
Mol. weight [g/mol]:	166.16
CAS:	1809-21-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	2.229		Crippen Method
mcvol	133.470	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	38.10	kJ/mol	392.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1809218&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

hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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