

Dibutyl hydrogen phosphite

Other names:	Dibutyl phosphite dibutyl phosphonate
Inchi:	InChI=1S/C8H19O3P/c1-3-5-7-10-12(9)11-8-6-4-2/h12H,3-8H2,1-2H3
InchiKey:	NFJPGAKRJKLOJK-UHFFFAOYSA-N
Formula:	C8H19O3P
SMILES:	CCCCO[PH](=O)OCCCC
Mol. weight [g/mol]:	194.21
CAS:	1809-19-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	3.010		Crippen Method
mcvol	161.650	ml/mol	McGowan Method
tb	546.08	K	Correlation of normal boiling points of dialkylalkyl phosphonates with topological indices on the gas chromatographic retention data

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	37.80	kJ/mol	368.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Correlation of normal boiling points of dialkylalkyl phosphonates with topological indices on the gas chromatographic retention data:	https://www.doi.org/10.1016/j.tca.2014.11.027
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1809194&Units=SI

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
tb:	Normal Boiling Point Temperature

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