

DIETHYL ETHYLPHOSPHONATE

Other names:	Diethyl ethylphosphonate Diethyl ethanephosphonate Amgard v 490 Diethoxyethylphosphine oxide Ethanephosphonic acid, diethyl ester
Inchi:	InChI=1S/C6H15O3P/c1-4-8-10(7,6-3)9-5-2/h4-6H2,1-3H3
InchiKey:	AATNZNJRDOVKDD-UHFFFAOYSA-N
Formula:	C6H15O3P
SMILES:	CCOP(=O)(CC)OCC
Mol. weight [g/mol]:	166.16

Physical Properties

Property code	Value	Unit	Source
hvap	59.67	kJ/mol	Cheméo Relay (1.0)
ie	9.73	eV	Cheméo Relay (1.0)
log10ws	0.07		Cheméo Relay (1.0)
logp	2.272		Crippen Method
mcvol	133.470	ml/mol	McGowan Method
tb	487.84	K	Cheméo Relay (1.0)
tf	212.98	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78386&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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