Methylphosphonic acid, dihexyl ester

Other names:	Methylphosphonic acid, dihexyl ester
	Phosphonic acid, P-methyl-, dihexyl ester
	Phosphonic acid, methyl-, O,O-dihexyl ester
Inchi:	InChI=1S/C13H29O3P/c1-4-6-8-10-12-15-17(3,14)16-13-11-9-7-5-2/h4-13H2,1-3H3
InchiKey:	XMEOPSOYUNXCJQ-UHFFFAOYSA-N
Formula:	C13H29O3P
SMILES:	CCCCCCOP(C)(=O)OCCCCCC
Mol. weight [g/mol]:	264.35

Physical Properties

Property code	Value	Unit	Source
af	0.7485		Cheméo Relay (1.0)
gf	-290.19	kJ/mol	Cheméo Relay (1.0, beta)
hf	-823.06	kJ/mol	Cheméo Relay (1.0)
hvap	85.98	kJ/mol	Cheméo Relay (1.0)
ie	9.84	eV	Cheméo Relay (1.0)
log10ws	-3.86		Cheméo Relay (1.0)
logp	5.003		Crippen Method
mcvol	232.100	ml/mol	McGowan Method
pc	1745.95	kPa	Cheméo Relay (1.0, beta)
tb	582.30	K	Cheméo Relay (1.0)
tc	716.35	K	Cheméo Relay (1.0)
tf	239.66	K	Cheméo Relay (1.0)
vc	0.906	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77304633&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume