Phosphonic acid, trimethylenedi-, tetraethyl ester

Other names: Phosphonic acid, trimethylenedi-, tetraethyl ester
Propane-1,3-diphosphonic acid, tetraethyl ester
Tetraethyl propane-1,3-diphosphonate

Inchi: InChI=1S/C11H26O6P2/c1-5-14-18(12,15-6-2)10-9-11-19(13,16-7-3)17-8-4/h5-11H2,1-4

InchiKey: LJQJJGQRJQSYQN-UHFFFAOYSA-N

Formula: C11H26O6P2

SMILES: CCOP(=O)(CCCP(=O)(OCC)OCC)OCC

Mol. weight [g/mol]: 316.27

Physical Properties

Property code	Value	Unit	Source
hvap	88.67	kJ/mol	Cheméo Relay (1.0)
ie	9.20	eV	Cheméo Relay (1.0)
log10ws	-0.96		Cheméo Relay (1.0)
logp	3.909		Crippen Method
mcvol	241.990	ml/mol	McGowan Method
tb	626.28	K	Cheméo Relay (1.0)
tf	237.34	K	Cheméo Relay (1.0)

Sources

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=C22401258&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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