Tetraethyl dimethylaminomethylene diphosphonate

Other names: Phosphonic acid, [(dimethylamino)methylene]bis-, tetraethyl ester
tetraethyl [(dimethylamino)methylene]bisphosphonate
Inchi: InChI=1S/C11H27NO6P2/c1-7-15-19(13,16-8-2)11(12(5)6)20(14,17-9-3)18-10-4/h11H,7-
InchiKey: SQDDGOVNJMIFFT-UHFFFAOYSA-N
Formula: C11H27NO6P2
SMILES: CCOP(=O)(OCC)C(N(C)C)P(=O)(OCC)OCC
Mol. weight [g/mol]: 331.29

Physical Properties

Property code	Value	Unit	Source
hvap	81.91	kJ/mol	Cheméo Relay (1.0)
ie	8.31	eV	Cheméo Relay (1.0)
log10ws	-1.51		Cheméo Relay (1.0)
logp	3.364		Crippen Method
mcvol	251.970	ml/mol	McGowan Method
tb	603.73	K	Cheméo Relay (1.0)
tf	237.80	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18855522&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):
Cheméo Relay (1.0, beta):

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