Methylenebis(phosphonic acid), tetraisopropyl ester

Other names: tetra-i-Propylmethylenediphosphonate
Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester
Methylenediphosphonic acid tetraisopropyl ester
Phosphonic acid, methylenedi-, tetraisopropyl ester
tetraisopropyl methylenebisphosphonate

Inchi: InChI=1S/C13H30O6P2/c1-10(2)16-20(14,17-11(3)4)9-21(15,18-12(5)6)19-13(7)8/h10-1

InchiKey: ODTQUKVFOLFLIQ-UHFFFAOYSA-N

Formula: C13H30O6P2

SMILES: CC(C)OP(=O)(CP(=O)(OC(C)C)OC(C)C)OC(C)C

Mol. weight [g/mol]: 344.32

Physical Properties

Property code	Value	Unit	Source
hvap	83.22	kJ/mol	Cheméo Relay (1.0)
logp	5.030		Crippen Method
mcvol	270.170	ml/mol	McGowan Method

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1660953&Units=SI

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

Legend

hvap: Enthalpy of vaporization at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume