ISOBUTYL METHYLPHOSPHONIC ACID, TMS DERIVATIVE

Other names: Methylphosphonic acid, isobutyl ester, TMS
Methylphosphonic acid, isobutyl trimethylsilyl ester
Methylphosphonic acid, mono-isobutyl ester, TMS

Inchi: InChI=1S/C8H21O3PSi/c1-8(2)7-10-12(3,9)11-13(4,5)6/h8H,7H2,1-6H3

InchiKey: YKENHQTWUXRYMG-UHFFFAOYSA-N

Formula: C8H21O3PSi

SMILES: CC(C)COP(C)(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 224.31

Physical Properties

Property code	Value	Unit	Source
hvap	57.86	kJ/mol	Cheméo Relay (1.0)
logp	3.333		Crippen Method
rinpol	1214.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1221.00		NIST Webbook
tb	498.77	K	Cheméo Relay (1.0)

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=C199116091&Units=SI

Legend

hvap: Enthalpy of vaporization at standard conditions

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature