

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

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