4-METHOXYPHENYLPYRUVIC ACID DITMS

Other names: 4-Methoxyphenylpyruvic acid, di-TMS
Phenylpyruvic acid, 4-methoxy, TMS
Inchi: InChI=1S/C16H26O4Si2/c1-18-14-10-8-13(9-11-14)12-15(19-21(2,3)4)16(17)20-22(5,6)7
InchiKey: IAKVNQLFHQCXOF-NTCAYCPXSA-N
Formula: C16H26O4Si2
SMILES: COc1ccc(/C=C(/O[Si](C)(C)C)C(=O)O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 338.55

Physical Properties

Property code	Value	Unit	Source
hvap	79.15	kJ/mol	Cheméo Relay (1.0)
ie	7.95	eV	Cheméo Relay (1.0)
log10ws	-3.93		Cheméo Relay (1.0)
logp	4.266		Crippen Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook
tb	616.12	K	Cheméo Relay (1.0)
tf	349.02	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750692&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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