ANISURIC ACID DITMS

Other names: Hippuric acid, 4-methoxy, TMS, # 1
Anisuric acid, bis(o
Inchi: InChI=1S/C16H27NO4Si2/c1-19-14-10-8-13(9-11-14)16(21-23(5,6)7)17-12-15(18)20-22(
InchiKey: NXIWRJOFVJVVCY-UHFFFAOYSA-N
Formula: C16H27NO4Si2
SMILES: COc1ccc(C(=NCC(=O)O[Si](C)(C)C)O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 353.57

Physical Properties

Property code	Value	Unit	Source
hf	-841.98	kJ/mol	Cheméo Relay (1.0)
hvap	83.19	kJ/mol	Cheméo Relay (1.0)
ie	8.07	eV	Cheméo Relay (1.0)
log10ws	-3.35		Cheméo Relay (1.0)
logp	3.671		Crippen Method
rinpol	2033.00		NIST Webbook
tb	609.29	K	Cheméo Relay (1.0)
tf	324.68	K	Cheméo Relay (1.0)

Sources

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=U71678&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions
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