Benzoic acid, 4-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Inchi: InChI=1S/C13H22O3Si2/c1-17(2,3)15-12-9-7-11(8-10-12)13(14)16-18(4,5)6/h7-10H,1-6H

InchiKey: XVCXIVAVMFNKDH-UHFFFAOYSA-N

Formula: C13H22O3Si2

SMILES: C[Si](C)(C)OC(=O)c1ccc(O[Si](C)(C)C)cc1

Mol. weight [g/mol]: 282.49

Physical Properties

Property code	Value	Unit	Source
hf	-750.74	kJ/mol	Cheméo Relay (1.0)
hvap	70.28	kJ/mol	Cheméo Relay (1.0)
ie	9.05	eV	Cheméo Relay (1.0)
log10ws	-3.49		Cheméo Relay (1.0)
logp	3.892		Crippen Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1620.50		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1620.50		NIST Webbook
rinpol	1628.60		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1628.60		NIST Webbook
tb	557.80	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078139&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

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