Benzoic acid, 3-methoxy-, trimethylsilyl ester

Other names: Benzoic acid, 3-methoxy, TMS
Inchi: InChI=1S/C11H16O3Si/c1-13-10-7-5-6-9(8-10)11(12)14-15(2,3)4/h5-8H,1-4H3
InchiKey: PPUSJGXNIQTKKU-UHFFFAOYSA-N
Formula: C11H16O3Si
SMILES: COc1cccc(C(=O)O[Si](C)(C)C)c1
Mol. weight [g/mol]: 224.33
CAS: 959111-51-4

Physical Properties

Property code	Value	Unit	Source
hf	-587.29	kJ/mol	Cheméo Relay (1.0)
hvap	71.44	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	2.687		Crippen Method
pc	1785.55	kPa	Cheméo Relay (1.0, beta)
rinpol	1485.00		NIST Webbook
rinpol	1455.00		NIST Webbook
tb	544.93	K	Cheméo Relay (1.0)
tc	725.35	K	Cheméo Relay (1.0)
tf	271.42	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=C959111514&Units=SI

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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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