Thiosalicylic acid, trimethylsilyl ester

Inchi: InChI=1S/C10H14O2SSi/c1-14(2,3)12-10(11)8-6-4-5-7-9(8)13/h4-7,13H,1-3H3
InchiKey: WZLZLYXCZVEIFB-UHFFFAOYSA-N
Formula: C10H14O2SSi
SMILES: C[Si](C)(C)OC(=O)c1ccccc1S
Mol. weight [g/mol]: 226.37

Physical Properties

Property code	Value	Unit	Source
hf	-444.09	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	Cheméo Relay (1.0)
log10ws	-3.32		Cheméo Relay (1.0)
logp	2.967		Crippen Method
pc	2148.83	kPa	Cheméo Relay (1.0, beta)
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	546.28	K	Cheméo Relay (1.0)
tf	289.46	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=U374596&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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
tf:	Normal melting (fusion) point

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