PHENOL TBDMS

Other names: Phenol, DMTBS
Phenol, tbdms derivative
Inchi: InChI=1S/C12H20OSi/c1-12(2,3)14(4,5)13-11-9-7-6-8-10-11/h6-10H,1-5H3
InchiKey: CLMZYPRKIYEXFB-UHFFFAOYSA-N
Formula: C12H20OSi
SMILES: CC(C)(C)[Si](C)(C)Oc1ccccc1
Mol. weight [g/mol]: 208.38

Physical Properties

Property code	Value	Unit	Source
hf	-281.77	kJ/mol	Cheméo Relay (1.0)
hvap	55.07	kJ/mol	Cheméo Relay (1.0)
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-3.17		Cheméo Relay (1.0)
logp	4.071		Crippen Method
pc	2298.92	kPa	Cheméo Relay (1.0, beta)
rinpol	1260.00		NIST Webbook
tb	503.07	K	Cheméo Relay (1.0)
tf	306.56	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U331820&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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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