1-Dimethyl(tert-butyl)silyloxy-3-methylbenzene

Other names:	1-Dimethyl(tert-butyl)silyloxy-3-methylbenzene
	m-Cresol, TBDMS
	Phenol, 3-methyl, DMTBS
	tert-Butyldimethylsilyl 3-methylphenyl ether
	M-cresol, tbdms derivative
Inchi:	InChI=1S/C13H22OSi/c1-11-8-7-9-12(10-11)14-15(5,6)13(2,3)4/h7-10H,1-6H3
InchiKey:	HBUBRNBOYWHGHQ-UHFFFAOYSA-N
Formula:	C13H22OSi
SMILES:	Cc1cccc(O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	222.40

Physical Properties

Property code	Value	Unit	Source
af	0.4503		Cheméo Relay (1.0)
gf	43.16	kJ/mol	Cheméo Relay (1.0, beta)
hf	-318.84	kJ/mol	Cheméo Relay (1.0)
hvap	55.70	kJ/mol	Cheméo Relay (1.0)
ie	8.23	eV	Cheméo Relay (1.0)
log10ws	-3.62		Cheméo Relay (1.0)
logp	4.379		Crippen Method
pc	2099.39	kPa	Cheméo Relay (1.0, beta)
rinpol	1356.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1356.00		NIST Webbook
tb	520.68	K	Cheméo Relay (1.0)
tc	725.38	K	Cheméo Relay (1.0)
tf	300.01	K	Cheméo Relay (1.0)
vc	0.724	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62790754&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

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
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
vc:	Critical Volume