

2-CRESOL TBDMS

Other names:	o-cresol, TBDMS O-cresol, tbdms derivative
Inchi:	InChI=1S/C13H22OSi/c1-11-9-7-8-10-12(11)14-15(5,6)13(2,3)4/h7-10H,1-6H3
InchiKey:	KMGYVHNBKRHULS-UHFFFAOYSA-N
Formula:	C13H22OSi
SMILES:	Cc1ccccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	222.40

Physical Properties

Property code	Value	Unit	Source
ie	8.25	eV	Cheméo Relay (1.0)
log10ws	-3.40		Cheméo Relay (1.0)
logp	4.379		Crippen Method
tb	512.92	K	Cheméo Relay (1.0)
tc	724.24	K	Cheméo Relay (1.0)
tf	294.55	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U331834&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point

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