6,7-DIHYDROXYCOUMARIN DI-TMS

Other names: Coumarin, 6,7-dihydroxy-, TMS
Aesculetin, TMS
Coumarin, 6,7-bis-trimethylsilyloxy
Inchi: InChI=1S/C15H22O4Si2/c1-20(2,3)18-13-9-11-7-8-15(16)17-12(11)10-14(13)19-21(4,5)6
InchiKey: KATLNZVTBBAXMH-UHFFFAOYSA-N
Formula: C15H22O4Si2
SMILES: C[Si](C)(C)Oc1cc2ccc(=O)oc2cc1O[Si](C)(C)C
Mol. weight [g/mol]: 322.51

Physical Properties

Property code	Value	Unit	Source
hf	-772.52	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-3.82		Cheméo Relay (1.0)
logp	4.220		Crippen Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
tb	646.67	K	Cheméo Relay (1.0)
tf	405.79	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U108963&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

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point