

Acenaphthene-cis-9,10-diol, DTBS

Inchi: InChI=1S/C20H26O2Si/c1-19(2,3)23(20(4,5)6)21-17-14-11-7-9-13-10-8-12-15(16(13)14)
InchiKey: BKYXICPAAUBOIR-HDICACEKSA-N
Formula: C20H26O2Si
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC2c3cccc4cccc(c34)C2O1
Mol. weight [g/mol]: 326.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	6.025		Crippen Method
rinpol	2070.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R115287&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/33-462-2/Acenaphthene-cis-9-10-diol-DTBS.pdf>

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