

trans-2,3-Dimethylacrylic acid, tert-butyldimethylsilyl ester

Other names: Tiglic acid, tbdms derivative
Inchi: InChI=1S/C11H22O2Si/c1-8-9(2)10(12)13-14(6,7)11(3,4)5/h8H,1-7H3/b9-8+
InchiKey: DYOOAKQETGCZTG-CMDGGOBGSA-N
Formula: C₁₁H₂₂O₂Si
SMILES: CC=C(C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 214.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.19		Crippen Method
logp	3.501		Crippen Method
rinpol	1232.60		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1232.60		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352568&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/42-762-9/trans-2-3-Dimethylacrylic-acid-tert-butyldimethylsilyl-ester.pdf>

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