

Brigalow ketol, TMS

Inchi: InChI=1S/C15H20O3/c1-10(2)8-13(16)14-11(3)4-6-15(14,17)12-5-7-18-9-12/h5,7-9,11,14
InchiKey: MZISRFGDZVZINJ-UHFFFAOYSA-N
Formula: C15H20O3
SMILES: CC(C)=CC(=O)C1C(C)CCC1(O)c1ccoc1
Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.75		Crippen Method
logp	3.049		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
rinpol	1768.00		NIST Webbook
rinpol	1768.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R584782&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/20-570-6/Brigalow-ketol-TMS.pdf>

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