

2-((3,3-Dimethyloxiran-2-yl)methyl)-3-methylfuran

Inchi: InChI=1S/C10H14O2/c1-7-4-5-11-8(7)6-9-10(2,3)12-9/h4-5,9H,6H2,1-3H3
InchiKey: BVTAXWVSMPSFL-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: Cc1ccoc1CC1OC1(C)C
Mol. weight [g/mol]: 166.22
CAS: 92356-06-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.95		Crippen Method
logp	2.308		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
rinpol	1177.20		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1177.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C92356064&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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