

(R)-1,5,8-Trimethyl-6,7,8,9-tetrahydronaphtho[2,1-

Inchi: InChI=1S/C15H18O/c1-9-4-5-12-10(2)7-14-15(13(12)6-9)11(3)8-16-14/h7-9H,4-6H2,1-3H
InchiKey: GWQCNWWIXOLIAV-SECBINFHSA-N
Formula: C15H18O
SMILES: Cc1cc2occ(C)c2c2c1CCC(C)C2
Mol. weight [g/mol]: 214.30
CAS: 59462-26-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.64		Crippen Method
logp	4.174		Crippen Method
mcvol	178.300	ml/mol	McGowan Method
rinpol	1860.80		NIST Webbook
rinpol	1860.80		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C59462269&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/79-392-0/R-1-5-8-Trimethyl-6-7-8-9-tetrahydronaphtho-2-1-b-furan.pdf>

Generated by Cheméo on 2024-04-25 05:57:05.62657161 +0000 UTC m=+16313874.547148928.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.