

Glechomafuran

Inchi: InChI=1S/C15H20O3/c1-9-8-16-11-7-15(3)12(17-15)4-5-14(2)13(18-14)6-10(9)11/h8,12-14
InchiKey: FNQFNSGVMLMZNV-XGUBFFRZSA-N
Formula: C15H20O3
SMILES: Cc1coc2c1CC1OC1(C)CCC1OC1(C)C2
Mol. weight [g/mol]: 248.32
CAS: 38146-67-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.10		Crippen Method
logp	2.782		Crippen Method
mcvol	187.780	ml/mol	McGowan Method
ripol	2854.00		NIST Webbook
ripol	2854.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C38146677&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
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/92-956-9/Glechomafuran.pdf>

Generated by Cheméo on 2024-04-25 18:47:36.936672641 +0000 UTC m=+16360105.857249952.

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