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-
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/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
ripol: Polar retention indices