5,6-seco-6,7-Furoeudesman-5-one

Inchi: InChI=1S/C15H22O2/c1-11-5-4-7-15(3,14(11)16)8-6-13-10-17-9-12(13)2/h9-11H,4-8H2,1
InchiKey: IOEWOOAPVQGVLB-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: Cc1cocc1CCC1(C)CCCC(C)C1=O
Mol. weight [g/mol]: 234.33
CAS: 311351-17-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.52		Crippen Method
logp	3.916		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
rinpol	1735.20		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1735.20		NIST Webbook
rinpol	1704.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C311351174&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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