

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,
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

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