

atractylone

Other names:	Atractylon
Inchi:	InChI=1S/C15H20O/c1-10-5-4-6-15(3)8-14-12(7-13(10)15)11(2)9-16-14/h9,13H,1,4-8H2,
InchiKey:	TYPSPVDGIQAOBAD-WUJWULDRSA-N
Formula:	C15H20O
SMILES:	C=C1CCCC2(C)Cc3occ(C)c3CC12
Mol. weight [g/mol]:	216.32
CAS:	6989-21-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.96		Crippen Method
logp	4.049		Crippen Method
mcvol	182.600	ml/mol	McGowan Method
rinpol	1669.30		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1652.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6989215&Units=SI

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/60-990-6/atractylone.pdf>

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