

Atractylodin

Inchi:	InChI=1S/C13H10O/c1-2-3-4-5-6-7-8-10-13-11-9-12-14-13/h2-3,8-12H,1H3/b3-2+,10-8+
InchiKey:	GRBKWAXRYIITKG-QFMFQGICSA-N
Formula:	C13H10O
SMILES:	CC=CC#CC#CC=Cc1cccc1
Mol. weight [g/mol]:	182.22
CAS:	55290-63-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.40		Crippen Method
logp	2.876		Crippen Method
mcvol	154.640	ml/mol	McGowan Method
rinpole	1686.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55290636&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
rinpole:	Non-polar retention indices

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