

cis-threo-Davanafuran

Other names:	(Z)-threo-davanofuran
Inchi:	InChI=1S/C14H20O2/c1-5-14(4)9-8-13(16-14)11(3)12-7-6-10(2)15-12/h5-7,11,13H,1,8-9
InchiKey:	RZQBGGYIEUNQIV-IACUBPJLSA-N
Formula:	C14H20O2
SMILES:	C=CC1(C)CCC(C(C)c2ccc(C)o2)O1
Mol. weight [g/mol]:	220.31
CAS:	54750-65-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.44		Crippen Method
logp	3.815		Crippen Method
mcvol	185.240	ml/mol	McGowan Method
rinpol	1409.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1414.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54750651&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

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