

Furfurylamphetamine

Inchi: InChI=1S/C14H17NO/c1-12(10-13-6-3-2-4-7-13)15-11-14-8-5-9-16-14/h2-9,12,15H,10-1
InchiKey: XWWSVBIGONHVQI-UHFFFAOYSA-N
Formula: C14H17NO
SMILES: CC(Cc1ccccc1)NCc1ccco1
Mol. weight [g/mol]: 215.29
CAS: 23656-74-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.26		Crippen Method
logp	3.000		Crippen Method
mcvol	180.750	ml/mol	McGowan Method
rinpol	1617.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1630.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2281.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2271.00		NIST Webbook

Sources

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=C23656748&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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