

2-Tridecyfuran

Inchi: InChI=1S/C17H30O/c1-2-3-4-5-6-7-8-9-10-11-12-14-17-15-13-16-18-17/h13,15-16H,2-12H
InchiKey: LFPGJDSJDXWCIJ-UHFFFAOYSA-N
Formula: C17H30O
SMILES: CCCCCCCCCCCCCc1ccco1
Mol. weight [g/mol]: 250.42
CAS: 25346-22-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.61		Crippen Method
logp	6.133		Crippen Method
mcvol	236.800	ml/mol	McGowan Method
rinpol	1802.40		NIST Webbook
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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=C25346229&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/74-517-6/2-Tridecyfuran.pdf>

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