

2-Dodecylfuran

Inchi: InChI=1S/C16H28O/c1-2-3-4-5-6-7-8-9-10-11-13-16-14-12-15-17-16/h12,14-15H,2-11,13
InchiKey: YCHOIEWPPPNUFM-UHFFFAOYSA-N
Formula: C16H28O
SMILES: CCCCCCCCCCCCc1ccco1
Mol. weight [g/mol]: 236.39
CAS: 75308-12-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.19		Crippen Method
logp	5.743		Crippen Method
mcvol	222.710	ml/mol	McGowan Method
rinpola	1703.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C75308122&Units=SI>
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>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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