

2-(6-Methylheptyl)furan

Inchi: InChI=1S/C12H20O/c1-11(2)7-4-3-5-8-12-9-6-10-13-12/h6,9-11H,3-5,7-8H2,1-2H3
InchiKey: UFRGZBAEVLDOKG-UHFFFAOYSA-N
Formula: C12H20O
SMILES: CC(C)CCCCC1CCCO1
Mol. weight [g/mol]: 180.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.28		Crippen Method
logp	4.038		Crippen Method
mcvol	166.350	ml/mol	McGowan Method
rinpol	1265.00		NIST Webbook
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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=R412612&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/27-495-3/2-6-Methylheptyl-furan.pdf>

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