

furfuryl hexyl ketone

Inchi: InChI=1S/C11H16O2/c1-2-3-4-6-10(12)9-11-7-5-8-13-11/h5,7-8H,2-4,6,9H2,1H3
InchiKey: GLSSAJXXNUOYOG-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CCCCCC(=O)Cc1cccO1
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.38		Crippen Method
logp	2.971		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
ripol	1913.00		NIST Webbook
ripol	1913.00		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=R315650&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/86-360-7/furfuryl-hexyl-ketone.pdf>

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