

Octanoic acid, 2-furanylmethyl ester

Other names: Furfuryl octanoate
Inchi: InChI=1S/C13H20O3/c1-2-3-4-5-6-9-13(14)16-11-12-8-7-10-15-12/h7-8,10H,2-6,9,11H2,
InchiKey: JNlWCVWKECYDSV-UHFFFAOYSA-N
Formula: C13H20O3
SMILES: CCCCCCCC(=O)OCc1ccco1
Mol. weight [g/mol]: 224.30
CAS: 39252-03-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.30		Crippen Method
logp	3.683		Crippen Method
mcvol	187.880	ml/mol	McGowan Method
rinpol	1543.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C39252034&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
rinpol: Non-polar retention indices

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