

N-Amyl furylpropionate

Other names:	Amyl furfuryl propionate
Inchi:	InChI=1S/C12H18O3/c1-2-3-4-9-15-12(13)8-7-11-6-5-10-14-11/h5-6,10H,2-4,7-9H2,1H3
InchiKey:	MRNLJBGPIOBGFP-UHFFFAOYSA-N
Formula:	C12H18O3
SMILES:	CCCCCOC(=O)CCc1ccco1
Mol. weight [g/mol]:	210.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.38		Crippen Method
logp	2.946		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
ripol	1947.00		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=U284966&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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