

2-Furancarboxylic acid, hexyl ester

Other names:	Hexyl 2-furoate Hexyl furoate
Inchi:	InChI=1S/C11H16O3/c1-2-3-4-5-8-14-11(12)10-7-6-9-13-10/h6-7,9H,2-5,8H2,1H3
InchiKey:	KMLFVAGUWNPADU-UHFFFAOYSA-N
Formula:	C11H16O3
SMILES:	CCCCCOC(=O)c1ccco1
Mol. weight [g/mol]:	196.24
CAS:	39251-86-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.54		Crippen Method
logp	3.017		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
ripol	1998.00		NIST Webbook
ripol	1998.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39251860&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices

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