

1-Heptanone, 1-(2-furanyl)-

Other names:	2-Heptanoylfuran Furan, 2-heptanoyl
Inchi:	InChI=1S/C11H16O2/c1-2-3-4-5-7-10(12)11-8-6-9-13-11/h6,8-9H,2-5,7H2,1H3
InchiKey:	BTNRWSUWLFXEL-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	CCCCCCC(=O)c1ccco1
Mol. weight [g/mol]:	180.24
CAS:	5466-40-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.96		Crippen Method
logp	3.433		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
ripol	1956.00		NIST Webbook
ripol	1956.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5466400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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