2-Hexanoylfuran

Other names:	2-Furyl n-pentyl ketone
	1-Hexanone, 1-(2-furanyl)-
	1-(2-Furyl)-1-hexanone
	Pentyl 2-furyl ketone
	Furan, 2-hexanoyl
	Pentyl furyl ketone
	1-(2-furyl)hexanone
Inchi:	InChI=1S/C10H14O2/c1-2-3-4-6-9(11)10-7-5-8-12-10/h5,7-8H,2-4,6H2,1H3
InchiKey:	YUAYWSBSIJVIBS-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CCCCCC(=O)c1ccco1
Mol. weight [g/mol]:	166.22
CAS:	14360-50-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.54		Crippen Method
logp	3.043		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1281.00		NIST Webbook
rinpol	1239.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	1850.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.00 ± 1.00	K	0.07	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14360500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure