

Furan, 2-hexyl-

Other names:	2-Hexylfuran 2-n-Hexylfuran
Inchi:	InChI=1S/C10H16O/c1-2-3-4-5-7-10-8-6-9-11-10/h6,8-9H,2-5,7H2,1H3
InchiKey:	XBLCAKKYMZVLPU-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CCCCCc1ccco1
Mol. weight [g/mol]:	152.23
CAS:	3777-70-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.68		Crippen Method
logp	3.402		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
rinpol	1097.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1086.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1316.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1345.00		NIST Webbook

ripol	1326.00	NIST Webbook
ripol	1345.00	NIST Webbook
ripol	1329.00	NIST Webbook
ripol	1323.00	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=C3777706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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