

2-n-Octylfuran

Other names:	Furan, 2-octyl- 2-Octylfuran
Inchi:	InChI=1S/C12H20O/c1-2-3-4-5-6-7-9-12-10-8-11-13-12/h8,10-11H,2-7,9H2,1H3
InchiKey:	RADIRWIUSSENFU-UHFFFAOYSA-N
Formula:	C12H20O
SMILES:	CCCCCCCCc1ccco1
Mol. weight [g/mol]:	180.29
CAS:	4179-38-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.52		Crippen Method
logp	4.183		Crippen Method
mcpol	166.350	ml/mol	McGowan Method
ripol	1281.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1520.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4179388&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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