

1-Octanone, 1-(2-thienyl)-

Other names:	2-Octanoylthiophene 1-(2-Thienyl)-1-octanone 2-n-Octanoylthiophene Thiophene, 2-octanoyl
Inchi:	InChI=1S/C12H18OS/c1-2-3-4-5-6-8-11(13)12-9-7-10-14-12/h7,9-10H,2-6,8H2,1H3
InchiKey:	QRJZCQOLJVIBDE-UHFFFAOYSA-N
Formula:	C12H18OS
SMILES:	CCCCCCCC(=O)c1cccs1
Mol. weight [g/mol]:	210.34
CAS:	30711-41-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.40		Crippen Method
logp	4.291		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
ripol	2313.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30711412&Units=SI

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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