

1-(2-furanyl)-3-butanone

Other names:	1-(2-furyl)-3-butanone 1-(2-Furyl)butan-3-one 2-Butanone, 4-(2-furyl)- 3-Butanone, 1-(2-furanyl) 4-(2-furyl)butan-2-one
Inchi:	InChI=1S/C8H10O2/c1-7(9)4-5-8-3-2-6-10-8/h2-3,6H,4-5H2,1H3
InchiKey:	GGJUJWSDTDBTLX-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	CC(=O)CCc1ccco1
Mol. weight [g/mol]:	138.16
CAS:	699-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.13		Crippen Method
logp	1.801		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
ripol	1089.00		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1059.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1057.00		NIST Webbook
ripol	1059.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1634.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1634.00		NIST Webbook
ripol	1625.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C699172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

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