

1-Propanone, 1-(2-furanyl)-

Other names:	1-Propanone, 1-(2-furyl)-
	Ethyl 2-furyl ketone
	Furyl ethyl ketone
	2-Furyl ethyl ketone
	2-Propionylfuran
	1-(2-Furanyl)-1-propanone
	1-Furan-2-yl-propan-1-one
	Ethyl furyl ketone
	1-(2-Furanyl)-propanone
	1-(2-furyl)-1-propanone
	1-(2-furyl)propan-1-one
Inchi:	InChI=1S/C7H8O2/c1-2-6(8)7-4-3-5-9-7/h3-5H,2H2,1H3
InchiKey:	HCPORNAVHSWTOJ-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	CCC(=O)c1ccco1
Mol. weight [g/mol]:	124.14
CAS:	3194-15-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	1.872		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpol	1019.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	977.00		NIST Webbook

rinpol	976.00	NIST Webbook
rinpol	1022.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	984.00	NIST Webbook
rinpol	983.00	NIST Webbook
rinpol	988.00	NIST Webbook
rinpol	984.00	NIST Webbook
rinpol	1008.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	1005.00	NIST Webbook
rinpol	987.00	NIST Webbook
rinpol	1008.00	NIST Webbook
rinpol	976.00	NIST Webbook
ripol	1560.00	NIST Webbook
ripol	1563.00	NIST Webbook
ripol	1571.00	NIST Webbook
ripol	1558.00	NIST Webbook
ripol	1563.00	NIST Webbook
ripol	1569.00	NIST Webbook
ripol	1563.00	NIST Webbook
ripol	1560.00	NIST Webbook
ripol	1565.00	NIST Webbook
ripol	1563.00	NIST Webbook
ripol	1560.00	NIST Webbook
ripol	1611.00	NIST Webbook
ripol	1564.00	NIST Webbook
ripol	1562.00	NIST Webbook
ripol	1562.00	NIST Webbook
ripol	1561.00	NIST Webbook
ripol	1560.00	NIST Webbook
ripol	1571.00	NIST Webbook
ripol	1557.00	NIST Webbook
ripol	1567.00	NIST Webbook
ripol	1554.00	NIST Webbook
ripol	1551.00	NIST Webbook
ripol	1565.00	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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=C3194158&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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