

«alpha»-Oxo-furan-2-acetonitrile

Other names:	2-Furanacetonitrile, «alpha»-oxo- 2-Furanglyoxylonitrile 2-furoyl cyanide
Inchi:	InChI=1S/C6H3NO2/c7-4-5(8)6-2-1-3-9-6/h1-3H
InchiKey:	BITJKGFKDMCINV-UHFFFAOYSA-N
Formula:	C6H3NO2
SMILES:	N#CC(=O)c1ccco1
Mol. weight [g/mol]:	121.09
CAS:	6047-91-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.73		Crippen Method
logp	0.986		Crippen Method
mcvol	84.760	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6047912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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