

5-Ethyl-2-furaldehyde

Other names:	5-Ethylfurfural 2-Furancarboxaldehyde, 5-ethyl- Furan-2-carboxaldehyde, 5-ethyl
Inchi:	InChI=1S/C7H8O2/c1-2-6-3-4-7(5-8)9-6/h3-5H,2H2,1H3
InchiKey:	XADGZBFXFWQHBDB-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	CCc1ccc(C=O)o1
Mol. weight [g/mol]:	124.14
CAS:	23074-10-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.25		Crippen Method
logp	1.655		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1641.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23074104&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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