

2-Furancarboxaldehyde, 5-[(5-methyl-2-furanyl)methyl]-

Other names:	2-(5-Methyl-2-furfuryl)-5-furfural
Inchi:	InChI=1S/C11H10O3/c1-8-2-3-9(13-8)6-10-4-5-11(7-12)14-10/h2-5,7H,6H2,1H3
InchiKey:	KWIASFUDUPQEGZ-UHFFFAOYSA-N
Formula:	C11H10O3
SMILES:	<chem>Cc1ccc(Cc2ccc(C=O)o2)o1</chem>
Mol. weight [g/mol]:	190.20
CAS:	34995-74-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.76		Crippen Method
logp	2.584		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
ripol	1541.00		NIST Webbook
ripol	2322.00		NIST Webbook
ripol	2362.00		NIST Webbook
ripol	2322.00		NIST Webbook
ripol	2374.00		NIST Webbook
ripol	2362.00		NIST Webbook
ripol	2363.00		NIST Webbook
ripol	2363.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34995749&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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