

3,4,5-trimethyl-2-furfural

Other names:	trimethylfurfural
Inchi:	InChI=1S/C8H10O2/c1-5-6(2)8(4-9)10-7(5)3/h4H,1-3H3
InchiKey:	MHDALBBSPUFMJD-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	<chem>Cc1oc(C=O)c(C)c1C</chem>
Mol. weight [g/mol]:	138.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.87		Crippen Method
logp	2.017		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
rinpol	1130.00		NIST Webbook
ripol	1766.00		NIST Webbook
ripol	1766.00		NIST Webbook

Sources

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=R238632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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