3-methyl-2-furfural

Other names:	3-Methylfurfural
	3-Methyl-2-formylfuran
Inchi:	InChI=1S/C6H6O2/c1-5-2-3-8-6(5)4-7/h2-4H,1H3
InchiKey:	DSMRYCOTKWYTRF-UHFFFAOYSA-N
Formula:	C6H6O2
SMILES:	Cc1ccoc1C=O
Mol. weight [g/mol]:	110.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	1.401		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
rinpol	938.00		NIST Webbook
rinpol	938.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1471.00		NIST Webbook
ripol	1472.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1462.00		NIST Webbook
ripol	1468.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R230183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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