4,5-Dimethyl-2-formylfuran

Inchi:	InChI=1S/C7H8O2/c1-5-3-7(4-8)9-6(5)2/h3-4H,1-2H3
InchiKey:	JPTPEPVCVXGNJM-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	Cc1cc(C=O)oc1C
Mol. weight [g/mol]:	124.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	1.709		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1078.00		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=R614878&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

Latest version available from:
https://www.chemeo.com/cid/92-796-7/4-5-Dimethyl-2-formylfuran.pdf

Generated by Cheméo on 2024-10-12 07:32:37.092353525 +0000 UTC m=+3299219.729322773.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.