Furan, 2,3,5-trimethyl-

Other names: 2,3,5-Trimethylfuran
Inchi: InChI=1S/C7H10O/c1-5-4-6(2)8-7(5)3/h4H,1-3H3
InchiKey: NJXZFRUNHWKHEC-UHFFFAOYSA-N
Formula: C7H10O
SMILES: Cc1cc(C)c(C)o1
Mol. weight [g/mol]: 110.15
CAS: 10504-04-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.63		Crippen Method
logp	2.205		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
rinpol	817.00		NIST Webbook
rinpol	803.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	809.00		NIST Webbook
ripol	1051.00		NIST Webbook
ripol	1036.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1036.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1038.00		NIST Webbook
ripol	1038.00		NIST Webbook
ripol	1065.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1056.00		NIST Webbook
tb	394.65 ± 1.00	K	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10504048&Units=SI

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
tb:	Normal Boiling Point Temperature

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