

5-Methylfuran-2-carboxylic acid methyl ester

Other names:	methyl 5-methylfuro-2-ate 2-Furancarboxylic acid, 5-methyl-, methyl ester
Inchi:	InChI=1S/C7H8O3/c1-5-3-4-6(10-5)7(8)9-2/h3-4H,1-2H3
InchiKey:	XBYZJUMTKHUJIY-UHFFFAOYSA-N
Formula:	C7H8O3
SMILES:	COC(=O)c1ccc(C)o1
Mol. weight [g/mol]:	140.14
CAS:	2527-96-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	1.375		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
ripol	1043.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1654.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.20	K	2.00	NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2527960&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
tbrp: Boiling point at reduced pressure

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