

Furoic acid, methyl ester

Other names:	Furancarboxylic acid, methyl ester methyl 2-furoate methyl furoate
Inchi:	InChI=1S/C6H6O3/c1-8-6(7)5-3-2-4-9-5/h2-4H,1H3
InchiKey:	HDJLSECJEQSPKW-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	<chem>COC(=O)c1ccco1</chem>
Mol. weight [g/mol]:	126.11
CAS:	1334-76-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	1.066		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
tb	455.10 ± 0.50	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1334765&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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