

Ethyl 3-furoate

Other names:	3-Furancarboxylic acid, ethyl ester
Inchi:	InChI=1S/C7H8O3/c1-2-10-7(8)6-3-4-9-5-6/h3-5H,2H2,1H3
InchiKey:	LOFDXZJSDVCYAS-UHFFFAOYSA-N
Formula:	C7H8O3
SMILES:	CCOC(=O)c1ccoc1
Mol. weight [g/mol]:	140.14
CAS:	614-98-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	1.456		Crippen Method
mccvol	103.340	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.20	K	4.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C614982&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

Latest version available from:

<https://www.cheméo.com/cid/41-694-6/Ethyl-3-furoate.pdf>

Generated by Cheméo on 2024-04-19 02:19:37.169632552 +0000 UTC m=+15782426.090209863.

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