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
mcvol	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/ci990307l
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