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

Physical Properties

Property code	Value	Unit	Source
af	0.4787		Cheméo Relay (1.0)
hf	-423.00	kJ/mol	Cheméo Relay (1.0)
hvap	53.21	kJ/mol	Cheméo Relay (1.0)
ie	9.25	eV	Cheméo Relay (1.0)
log10ws	-1.86		Cheméo Relay (1.0)
logp	1.456		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
pc	3246.12	kPa	Cheméo Relay (1.0, beta)
tb	463.80	K	Cheméo Relay (1.0)
tc	658.27	K	Cheméo Relay (1.0)
tf	254.34	K	Cheméo Relay (1.0)

Pressure Dependent Properties

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C614982&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point