ethyl furoate

Other names:	2-(Ethoxycarbonyl)furan
	2-Carboethoxyfuran
	2-Furoic acid, ethyl ester
	Ethyl 2-furancarboxylate
	Ethyl 2-furoate
	Ethyl 2-furylcarboxylate
	Ethyl furan-2-carboxylate
	Ethyl furoate
	Ethyl pyromucate
	Furan-2-carboxylic acid ethyl ester
	NSC 2304
Inchi:	InChI=1S/C7H8O3/c1-2-9-7(8)6-4-3-5-10-6/h3-5H,2H2,1H3
InchiKey:	NHXSTXWKZVAVOQ-UHFFFAOYSA-N
Formula:	C7H8O3
SMILES:	CCOC(=O)c1ccco1
Mol. weight [g/mol]:	140.14
CAS:	1335-40-6

Physical Properties

Property code	Value	Unit	Source
af	0.4865		Cheméo Relay (1.0)
hf	-427.73	kJ/mol	Cheméo Relay (1.0)
hvap	55.06	kJ/mol	Cheméo Relay (1.0)
ie	8.94	eV	Cheméo Relay (1.0)
log10ws	-1.83		Cheméo Relay (1.0)
logp	1.456		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
pc	3163.35	kPa	Cheméo Relay (1.0, beta)
rinpol	1056.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1059.00		NIST Webbook
tb	470.61	K	Cheméo Relay (1.0)
tc	651.71	K	Cheméo Relay (1.0)
tf	249.10	K	Cheméo Relay (1.0)

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1335406&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point