ETHYL 2-THIOPHENECARBOXYLATE

Other names: 2-Thiophenecarboxylic acid, ethyl ester
Ethyl 2-thenoate
Ethyl thiophene-2-carboxylate
Inchi: InChI=1S/C7H8O2S/c1-2-9-7(8)6-4-3-5-10-6/h3-5H,2H2,1H3
InchiKey: JZGZKRJVTIRPOK-UHFFFAOYSA-N
Formula: C7H8O2S
SMILES: CCOC(=O)c1cccs1
Mol. weight [g/mol]: 156.21

Physical Properties

Property code	Value	Unit	Source
af	0.4479		Cheméo Relay (1.0)
hf	-295.87	kJ/mol	Cheméo Relay (1.0)
hvap	56.60 ± 1.30	kJ/mol	NIST Webbook
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	-2.56		Cheméo Relay (1.0)
logp	1.925		Crippen Method
mcvol	113.820	ml/mol	McGowan Method
pc	3168.02	kPa	Cheméo Relay (1.0, beta)
tb	491.20	K	NIST Webbook
tc	687.25	K	Cheméo Relay (1.0)
tf	247.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	61.20	kJ/mol	298.15	Experimental redetermination of the gas-phase enthalpy of formation of ethyl 2-thiophenecarboxylate

Sources

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):	
Calorimetric study of methyl and ethyl 2-thiophenecarboxylates and ethyl 2-and 3-thiopheneacetates:	https://www.doi.org/10.1016/j.jct.2009.03.007
Experimental redetermination of the gas-phase enthalpy of formation of ethyl 2-thiophenecarboxylate:	https://www.doi.org/10.1016/j.jct.2012.09.007
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2810040&Units=SI

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point