

Thiophene-2-carboxylic acid ethyl ester

Other names:	2-Thiophenecarboxylic acid, ethyl ester Ethyl 2-thenoate Ethyl 2-thiophenecarboxylate 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]:	156.20
CAS:	2810-04-0

Physical Properties

Property code	Value	Unit	Source
hvap	56.60 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.925		Crippen Method
mvol	113.820	ml/mol	McGowan Method
tb	491.20	K	NIST Webbook

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2810040&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Calorimetric study of methyl and ethyl 2-thiophenecarboxylates and ethyl 2-mercaptoacetate. Experimental determination of the gas-phase enthalpy of formation of methyl and ethyl 2-thiophenecarboxylate: <https://www.doi.org/10.1016/j.jct.2009.03.007>
<https://www.doi.org/10.1016/j.jct.2012.09.007>
<http://link.springer.com/article/10.1007/BF02311772>

Legend

h_{vap}: Enthalpy of vaporization at standard conditions
h_{vap}t: Enthalpy of vaporization at a given temperature
log₁₀ws: Log₁₀ of Water solubility in mol/l
log_p: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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