Methyl-2-thiophene carboxylate

Other names:	2-(Carbomethoxy)thiophene
	2-(Methoxycarbonyl)thiophene
	2-Thiophenecarboxylic acid methyl ester
	Methyl thiophene-2-carboxylate
	Thiophenate methyl
	methyl 2-thiophenecarboxylate
	methyl thenoate
Inchi:	InChI=1S/C6H6O2S/c1-8-6(7)5-3-2-4-9-5/h2-4H,1H3
InchiKey:	PGBFYLVIMDQYMS-UHFFFAOYSA-N
Formula:	C6H6O2S
SMILES:	COC(=O)c1cccs1
Mol. weight [g/mol]:	142.18
CAS:	5380-42-7

Physical Properties

Property code	Value	Unit	Source
hvap	57.60 ± 1.20	kJ/mol	NIST Webbook
ie	9.22 ± 0.05	eV	NIST Webbook
ie	8.98 ± 0.05	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.535		Crippen Method
mcvol	99.730	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5380427&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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