

METHYL 2-THIOPHENECARBOXYLATE

Other names:	2-(Carbomethoxy)thiophene
	2-(Methoxycarbonyl)thiophene
	2-Thiophenecarboxylic acid methyl ester
	Methyl thiophene-2-carboxylate
	Thiophenate methyl
	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

Physical Properties

Property code	Value	Unit	Source
af	0.4156		Cheméo Relay (1.0)
hf	-252.24	kJ/mol	Cheméo Relay (1.0)
hvap	57.60 ± 1.20	kJ/mol	NIST Webbook
ie	8.98 ± 0.05	eV	NIST Webbook
ie	9.22 ± 0.05	eV	NIST Webbook
log10ws	-2.08		Cheméo Relay (1.0)
logp	1.535		Crippen Method
mcvol	99.730	ml/mol	McGowan Method
pc	3929.57	kPa	Cheméo Relay (1.0, beta)
tb	482.39	K	Cheméo Relay (1.0)
tc	681.92	K	Cheméo Relay (1.0)
tf	273.11	K	Cheméo Relay (1.0)
vc	0.355	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5380427&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):

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>

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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