Methyl tiglate

Other names:	Tiglic acid methyl ester
	2-Butenoic acid, 2-methyl-, methyl ester, (E)-
	Crotonic acid, 2-methyl-, methyl ester, (E)-
	Methyl (E)-2-methylcrotonate
	Methyl trans-2-methyl-2-butenoate
	2-Carbomethoxy-2-butene, (E)-
	Methyl «alpha»-methylcrotonate, trans-
	Methyl trans-2-methylcrotonate
	Methyl (2E)-2-methyl-2-butenoate
	2-Methylcrotonic acid, methyl ester, (E)-
	Methyl (E)-2-methyl-2-butenoate
	trans-2,3-Dimethylacrylic acid, methyl ester
	NSC 55277
	2-Butenoic acid, 2-methyl-, methyl ester, (2E)-
	2-Methylerotonic acid (Tiglicacid), methyl ester
	Methyl «alpha»-methylcrotonate
	methyl 2-methylcrotonate
Inchi:	InChI=1S/C6H10O2/c1-4-5(2)6(7)8-3/h4H,1-3H3/b5-4+
InchiKey:	YYJWBYNQJLBIGS-SNAWJCMRSA-N
Formula:	C6H10O2
SMILES:	CC=C(C)C(=O)OC
Mol. weight [g/mol]:	114.14
CAS:	6622-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-162.61	kJ/mol	Joback Method
hf	-304.54	kJ/mol	Joback Method
hfus	12.97	kJ/mol	Joback Method
hvap	38.14	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	863.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	868.00		NIST Webbook

rinpol	875.70		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	860.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1188.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1190.00		NIST Webbook
tb	417.01	K	Joback Method
tc	607.33	K	Joback Method
tf	210.50	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.26	J/mol×K	417.01	Joback Method
cpg	193.90	J/mol×K	448.73	Joback Method
cpg	203.14	J/mol×K	480.45	Joback Method
cpg	212.00	J/mol×K	512.17	Joback Method
cpg	220.47	J/mol×K	543.89	Joback Method
cpg	228.57	J/mol×K	575.61	Joback Method
cpg	236.31	J/mol×K	607.33	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.70	K	102.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6622760&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume