Tiglic acid

Other names:	(E)-2,3-Dimethylacrylic acid (E)-2-Methyl-2-butenoic acid (E)-2-Methylcrotonic acid (E)-2-methylbut-2-enoic acid 2-Butenoic acid, 2-methyl-, (2E)- 2-Butenoic acid, 2-methyl-, (E)- 2-methyl-(E)-2-butenoic acid Cevadic acid Crotonic acid, 2-methyl-, (E)- NSC 44235 Tiglic acid, (E)- Tiglinic acid trans-2,3-Dimethylacrylic acid trans-2-Methyl-2-butenoic acid trans-2-Methylcrotonic acid trans-Crotonic acid, 2-methyl- trans-«alpha»,«beta»-Dimethylacrylic Acid trans-Â«alphaÂ»,Â«betaÂ»-Dimethylacrylic Acid
Inchi:	InChI=1S/C5H8O2/c1-3-4(2)5(6)7/h3H,1-2H3,(H,6,7)/b4-3+
InchiKey:	UIERETOOQGIECD-ONEGZZNKSA-N
Formula:	C5H8O2
SMILES:	CC=C(C)C(=O)O
Mol. weight [g/mol]:	100.12
CAS:	80-59-1

Physical Properties

Property code	Value	Unit	Source
gf	-202.85	kJ/mol	Joback Method
hf	-303.91	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	50.19	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	1.037		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4857.97 ± 100.00	kPa	NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	941.00		NIST Webbook

rinpol	941.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1862.00		NIST Webbook
ripol	1867.00		NIST Webbook
ripol	1862.00		NIST Webbook
tb	471.70	K	NIST Webbook
tc	680.62 ± 3.00	K	NIST Webbook
tf	336.70 ± 1.50	K	NIST Webbook
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.62	J/mol×K	463.89	Joback Method
cpg	174.00	J/mol×K	494.57	Joback Method
cpg	181.01	J/mol×K	525.24	Joback Method
cpg	187.67	J/mol×K	555.92	Joback Method
cpg	193.97	J/mol×K	586.60	Joback Method
cpg	199.96	J/mol×K	617.27	Joback Method
cpg	205.63	J/mol×K	647.95	Joback Method
hvapt	61.20	kJ/mol	401.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33116e+01
Coeff. B	-2.76001e+03
Coeff. C	-1.54210e+02
Temperature range (K), min.	338.15
Temperature range (K), max.	499.21

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80591&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume