CH2=C(CH3)CH2COOH

Other names: 3-Methyl-3-butenoic acid
Inchi: InChI=1S/C5H8O2/c1-4(2)3-5(6)7/h1,3H2,2H3,(H,6,7)
InchiKey: IGRURXZWJCSNKU-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: C=C(C)CC(=O)O
Mol. weight [g/mol]: 100.12
CAS: 1617-31-8

Physical Properties

Property code	Value	Unit	Source
gf	-195.23	kJ/mol	Joback Method
hf	-295.70	kJ/mol	Joback Method
hfus	11.80	kJ/mol	Joback Method
hvap	49.56	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	1.037		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
tb	456.41	K	Joback Method
tc	635.70	K	Joback Method
tf	241.14	K	Joback Method
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.51	J/mol×K	456.41	Joback Method
cpg	174.73	J/mol×K	486.29	Joback Method
cpg	181.61	J/mol×K	516.17	Joback Method
cpg	188.18	J/mol×K	546.06	Joback Method
cpg	194.43	J/mol×K	575.94	Joback Method
cpg	200.39	J/mol×K	605.82	Joback Method
cpg	206.06	J/mol×K	635.70	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41304e+01
Coeff. B	-3.81714e+03
Coeff. C	-6.62500e+01
Temperature range (K), min.	342.00
Temperature range (K), max.	499.09

Sources

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=C1617318&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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume