2-Pentenoic acid, 2-methyl-

Other names: 2-Methyl-2-pentenoic acid
2-methylpent-2-en-1-oic acid
Inchi: InChI=1S/C6H10O2/c1-3-4-5(2)6(7)8/h4H,3H2,1-2H3,(H,7,8)/b5-4+
InchiKey: JJYWRQLLQAKNAD-SNAWJCMRSA-N
Formula: C6H10O2
SMILES: CCC=C(C)C(=O)O
Mol. weight [g/mol]: 114.14
CAS: 3142-72-1

Physical Properties

Property code	Value	Unit	Source
gf	-194.43	kJ/mol	Joback Method
hf	-324.55	kJ/mol	Joback Method
hfus	15.88	kJ/mol	Joback Method
hvap	52.41	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.427		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
rinpol	974.00		NIST Webbook
rinpol	974.00		NIST Webbook
ripol	1909.00		NIST Webbook
ripol	1909.00		NIST Webbook
tb	486.77	K	Joback Method
tc	669.02	K	Joback Method
tf	249.09	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.98	J/mol×K	486.77	Joback Method
cpg	214.52	J/mol×K	517.15	Joback Method
cpg	222.63	J/mol×K	547.52	Joback Method

cpg	230.34	J/mol×K	577.90	Joback Method
cpg	237.66	J/mol×K	608.27	Joback Method
cpg	244.62	J/mol×K	638.65	Joback Method
cpg	251.22	J/mol×K	669.02	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43961e+01
Coeff. B	-4.07452e+03
Coeff. C	-7.32000e+01
Temperature range (K), min.	362.00
Temperature range (K), max.	521.71

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3142721&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
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