2-methyl-3-pentenoic acid

Other names: 2-methylpent-3-en-1-oic acid
Inchi: InChI=1S/C6H10O2/c1-3-4-5(2)6(7)8/h3-5H,1-2H3,(H,7,8)/b4-3+
InchiKey: NFRJJFMXYKSRPK-ONEGZZNKSA-N
Formula: C6H10O2
SMILES: CC=CC(C)C(=O)O
Mol. weight [g/mol]: 114.14
CAS: 37674-63-8

Physical Properties

Property code	Value	Unit	Source
gf	-188.32	kJ/mol	Joback Method
hf	-320.04	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	51.94	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.283		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
ripol	1924.00		NIST Webbook
ripol	1924.00		NIST Webbook
tb	486.45	K	Joback Method
tc	669.30	K	Joback Method
tf	248.05	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.34	J/mol×K	486.45	Joback Method
cpg	215.01	J/mol×K	516.92	Joback Method
cpg	223.25	J/mol×K	547.40	Joback Method
cpg	231.07	J/mol×K	577.87	Joback Method
cpg	238.49	J/mol×K	608.35	Joback Method
cpg	245.53	J/mol×K	638.82	Joback Method

cpg	252.21	J/mol×K	669.30	Joback Method
dvisc	0.0452390	Pa×s	248.05	Joback Method
dvisc	0.0092323	Pa×s	287.78	Joback Method
dvisc	0.0027706	Pa×s	327.52	Joback Method
dvisc	0.0010788	Pa×s	367.25	Joback Method
dvisc	0.0005050	Pa×s	406.98	Joback Method
dvisc	0.0002706	Pa×s	446.72	Joback Method
dvisc	0.0001605	Pa×s	486.45	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41753e+01
Coeff. B	-3.99012e+03
Coeff. C	-7.24080e+01
Temperature range (K), min.	359.72
Temperature range (K), max.	522.56

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37674638&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume