2,2-Dimethylvaleric acid

Other names: 2,2-Dimethylpentanoic acid
Pentanoic acid, 2,2-dimethyl-
Valeric acid, 2,2-dimethyl-
«alpha»,«alpha»-Dimethylvaleric acid
Â«alphaÂ»,Â«alphaÂ»-Dimethylvaleric acid
Inchi: InChI=1S/C7H14O2/c1-4-5-7(2,3)6(8)9/h4-5H2,1-3H3,(H,8,9)
InchiKey: ZRYCZAWRXHAAPZ-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCCC(C)(C)C(=O)O
Mol. weight [g/mol]: 130.18
CAS: 1185-39-3

Physical Properties

Property code	Value	Unit	Source
gf	-254.84	kJ/mol	Joback Method
hf	-461.37	kJ/mol	Joback Method
hfus	12.16	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.897		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	470.00	K	NIST Webbook
tb	420.60 ± 2.00	K	NIST Webbook
tb	423.70 ± 2.00	K	NIST Webbook
tc	682.23	K	Joback Method
tf	281.82	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.88	J/mol×K	502.38	Joback Method
cpg	279.60	J/mol×K	532.36	Joback Method

cpg	289.76	J/mol×K	562.33	Joback Method
cpg	299.40	J/mol×K	592.31	Joback Method
cpg	308.52	J/mol×K	622.28	Joback Method
cpg	317.16	J/mol×K	652.26	Joback Method
cpg	325.33	J/mol×K	682.23	Joback Method
dvisc	0.0242619	Pa×s	281.82	Joback Method
dvisc	0.0066100	Pa×s	318.58	Joback Method
dvisc	0.0023568	Pa×s	355.34	Joback Method
dvisc	0.0010196	Pa×s	392.10	Joback Method
dvisc	0.0005092	Pa×s	428.86	Joback Method
dvisc	0.0002838	Pa×s	465.62	Joback Method
dvisc	0.0001723	Pa×s	502.38	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62687e+01
Coeff. B	-4.62077e+03
Coeff. C	-7.33810e+01
Temperature range (K), min.	362.52
Temperature range (K), max.	495.09

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=C1185393&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

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