2-hydroxy-3-methylvaleric acid

Other names: 2-Hydroxy-3-methylpentanoic acid
Inchi: InChI=1S/C6H12O3/c1-3-4(2)5(7)6(8)9/h4-5,7H,3H2,1-2H3,(H,8,9)
InchiKey: RILPIWOPNGRASR-UHFFFAOYSA-N
Formula: C6H12O3
SMILES: CCC(C)C(O)C(=O)O
Mol. weight [g/mol]: 132.16
CAS: 488-15-3

Physical Properties

Property code	Value	Unit	Source
gf	-407.80	kJ/mol	Joback Method
hf	-594.77	kJ/mol	Joback Method
hfus	14.02	kJ/mol	Joback Method
hvap	68.28	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.478		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
rinpol	1142.60		NIST Webbook
rinpol	1142.60		NIST Webbook
tb	574.03	K	Joback Method
tc	745.52	K	Joback Method
tf	298.95	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.65	J/mol×K	574.03	Joback Method
cpg	276.80	J/mol×K	602.61	Joback Method
cpg	284.57	J/mol×K	631.19	Joback Method
cpg	291.99	J/mol×K	659.77	Joback Method
cpg	299.06	J/mol×K	688.35	Joback Method
cpg	305.80	J/mol×K	716.93	Joback Method

cpg	312.20	J/mol×K	745.52	Joback Method
dvisc	0.0791815	Pa×s	298.95	Joback Method
dvisc	0.0100700	Pa×s	344.80	Joback Method
dvisc	0.0020780	Pa×s	390.64	Joback Method
dvisc	0.0005974	Pa×s	436.49	Joback Method
dvisc	0.0002177	Pa×s	482.34	Joback Method
dvisc	0.0000945	Pa×s	528.18	Joback Method
dvisc	0.0000469	Pa×s	574.03	Joback Method

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=C488153&Units=SI
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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