

4-hydroxy-3-methylpentanoic acid

Inchi:	InChI=1S/C6H12O3/c1-4(5(2)7)3-6(8)9/h4-5,7H,3H2,1-2H3,(H,8,9)
InchiKey:	BNTHHYUWQILHSA-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	CC(O)C(C)CC(=O)O
Mol. weight [g/mol]:	132.16

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
mvol	108.710	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
ripol	2642.00		NIST Webbook
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tb	574.03	K	Joback Method
tc	745.52	K	Joback Method
tf	298.95	K	Joback Method
vc	0.404	m ³ /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	Paxs	298.95	Joback Method

dvisc	0.0100700	Paxs	344.80	Joback Method
dvisc	0.0020780	Paxs	390.64	Joback Method
dvisc	0.0005974	Paxs	436.49	Joback Method
dvisc	0.0002177	Paxs	482.34	Joback Method
dvisc	0.0000945	Paxs	528.18	Joback Method
dvisc	0.0000469	Paxs	574.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R335030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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