2-Hydroxy-3-methylpentanoic 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

Physical Properties

Property code	Value	Unit	Source
af	0.7316		Cheméo Relay (1.0)
gf	-407.80	kJ/mol	Joback Method
hf	-692.06	kJ/mol	Cheméo Relay (1.0)
hfus	14.03	kJ/mol	Joback Method
hvap	77.66	kJ/mol	Cheméo Relay (1.0)
ie	10.34	eV	Cheméo Relay (1.0)
log10ws	0.04		Cheméo Relay (1.0)
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	471.86	K	Cheméo Relay (1.0)
tc	690.47	K	Cheméo Relay (1.0)
tf	309.40	K	Cheméo Relay (1.0)
vc	0.376	m3/kmol	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C488153&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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