

«alpha»-Hydroxyisobutyric acid, acetate

Inchi:	InChI=1S/C6H10O4/c1-4(7)10-6(2,3)5(8)9/h1-3H3,(H,8,9)
InchiKey:	NIWFXRKHWWKGFMT-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	CC(=O)OC(C)(C)C(=O)O
Mol. weight [g/mol]:	146.14

Physical Properties

Property code	Value	Unit	Source
gf	-497.18	kJ/mol	Joback Method
hf	-685.53	kJ/mol	Joback Method
hfus	12.36	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	0.413		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
rinpol	1092.00		NIST Webbook
tb	555.79	K	Joback Method
tc	745.30	K	Joback Method
tf	342.71	K	Joback Method
vc	0.409	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.74	J/mol×K	555.79	Joback Method
cpg	270.41	J/mol×K	587.37	Joback Method
cpg	278.62	J/mol×K	618.96	Joback Method
cpg	286.37	J/mol×K	650.54	Joback Method
cpg	293.68	J/mol×K	682.13	Joback Method
cpg	300.57	J/mol×K	713.71	Joback Method
cpg	307.03	J/mol×K	745.30	Joback Method
dvisc	0.0058366	Paxs	342.71	Joback Method
dvisc	0.0022681	Paxs	378.22	Joback Method

dvisc	0.0010366	Paxs	413.74	Joback Method
dvisc	0.0005362	Paxs	449.25	Joback Method
dvisc	0.0003055	Paxs	484.76	Joback Method
dvisc	0.0001880	Paxs	520.28	Joback Method
dvisc	0.0001230	Paxs	555.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374313&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
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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