

2-Hydroxyisocaproic acid, acetate

Inchi:	InChI=1S/C8H14O4/c1-5(2)4-7(8(10)11)12-6(3)9/h5,7H,4H2,1-3H3,(H,10,11)
InchiKey:	IQAAMERVQHMBU-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	CC(=O)OC(CC(C)C)C(=O)O
Mol. weight [g/mol]:	174.19

Physical Properties

Property code	Value	Unit	Source
gf	-488.06	kJ/mol	Joback Method
hf	-728.62	kJ/mol	Joback Method
hfus	17.90	kJ/mol	Joback Method
hvap	65.21	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	1.049		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinsol	1286.00		NIST Webbook
tb	603.90	K	Joback Method
tc	786.64	K	Joback Method
tf	332.83	K	Joback Method
vc	0.520	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.78	J/molxK	603.90	Joback Method
cpg	360.20	J/molxK	634.36	Joback Method
cpg	370.14	J/molxK	664.81	Joback Method
cpg	379.59	J/molxK	695.27	Joback Method
cpg	388.56	J/molxK	725.72	Joback Method
cpg	397.06	J/molxK	756.18	Joback Method
cpg	405.08	J/molxK	786.64	Joback Method
dvisc	0.0088194	Paxs	332.83	Joback Method
dvisc	0.0025337	Paxs	378.01	Joback Method

dvisc	0.0009500	Paxs	423.19	Joback Method
dvisc	0.0004304	Paxs	468.37	Joback Method
dvisc	0.0002242	Paxs	513.54	Joback Method
dvisc	0.0001297	Paxs	558.72	Joback Method
dvisc	0.0000815	Paxs	603.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374893&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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