

Alpha-hydroxy-isobutyric acid, n-butyl ester

Other names:	2-Hydroxyisobutyric acid, butylester
Inchi:	InChI=1S/C8H16O3/c1-4-5-6-11-7(9)8(2,3)10/h10H,4-6H2,1-3H3
InchiKey:	KDOLGPLJUMQYBO-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCCCOC(=O)C(C)(C)O
Mol. weight [g/mol]:	160.21
CAS:	816-50-2

Physical Properties

Property code	Value	Unit	Source
gf	-351.42	kJ/mol	Joback Method
hf	-614.23	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.101		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	547.68	K	Joback Method
tc	725.07	K	Joback Method
tf	315.32	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.31	J/molxK	725.07	Joback Method
cpg	336.80	J/molxK	547.68	Joback Method
cpg	348.18	J/molxK	577.24	Joback Method
cpg	359.02	J/molxK	606.81	Joback Method
cpg	369.33	J/molxK	636.37	Joback Method
cpg	379.14	J/molxK	665.94	Joback Method
cpg	388.47	J/molxK	695.50	Joback Method
dvisc	0.0001039	Paxs	547.68	Joback Method

dvisc	0.0099742	Paxs	315.32	Joback Method
dvisc	0.0030749	Paxs	354.05	Joback Method
dvisc	0.0011956	Paxs	392.77	Joback Method
dvisc	0.0005507	Paxs	431.50	Joback Method
dvisc	0.0002883	Paxs	470.23	Joback Method
dvisc	0.0001665	Paxs	508.95	Joback Method
hvapt	47.70	kJ/mol	421.00	NIST Webbook

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=C816502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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