

2-Hydroxyisocaproic acid, methyl ether, methyl ester

Inchi:	InChI=1S/C8H16O3/c1-6(2)5-7(10-3)8(9)11-4/h6-7H,5H2,1-4H3
InchiKey:	MRITUNXBFHKLSY-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	COC(=O)C(CC(C)C)OC
Mol. weight [g/mol]:	160.21

Physical Properties

Property code	Value	Unit	Source
gf	-327.32	kJ/mol	Joback Method
hf	-596.03	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	1.220		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinsol	1011.10		NIST Webbook
tb	480.27	K	Joback Method
tc	662.33	K	Joback Method
tf	244.31	K	Joback Method
vc	0.513	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.20	J/molxK	480.27	Joback Method
cpg	363.52	J/molxK	631.99	Joback Method
cpg	352.53	J/molxK	601.65	Joback Method
cpg	341.10	J/molxK	571.30	Joback Method
cpg	329.23	J/molxK	540.96	Joback Method
cpg	316.93	J/molxK	510.61	Joback Method
cpg	374.06	J/molxK	662.33	Joback Method
dvisc	0.0001926	Paxs	480.27	Joback Method
dvisc	0.0002606	Paxs	440.94	Joback Method

dvisc	0.0003743	Paxs	401.62	Joback Method
dvisc	0.0005814	Paxs	362.29	Joback Method
dvisc	0.0010055	Paxs	322.96	Joback Method
dvisc	0.0020240	Paxs	283.64	Joback Method
dvisc	0.0051039	Paxs	244.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332756&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

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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