Pentanoic acid, 3-hydroxy-, methyl ester

Other names: Methyl 3-hydroxypentanoate
Inchi: InChI=1S/C6H12O3/c1-3-5(7)4-6(8)9-2/h5,7H,3-4H2,1-2H3
InchiKey: XHFXKKFVUDJSPJ-UHFFFAOYSA-N
Formula: C6H12O3
SMILES: CCC(O)CC(=O)OC
Mol. weight [g/mol]: 132.16
CAS: 56009-31-5

Physical Properties

Property code	Value	Unit	Source
gf	-373.54	kJ/mol	Joback Method
hf	-569.48	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.320		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
ripol	1540.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1540.00		NIST Webbook
tb	504.71	K	Joback Method
tc	679.05	K	Joback Method
tf	275.36	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.76	J/mol×K	504.71	Joback Method
cpg	287.86	J/mol×K	649.99	Joback Method
cpg	280.10	J/mol×K	620.94	Joback Method
cpg	272.02	J/mol×K	591.88	Joback Method
cpg	263.60	J/mol×K	562.82	Joback Method

cpg	254.84	J/mol×K	533.77	Joback Method
cpg	295.29	J/mol×K	679.05	Joback Method
dvisc	0.0001487	Pa×s	504.71	Joback Method
dvisc	0.0002420	Pa×s	466.49	Joback Method
dvisc	0.0004297	Pa×s	428.26	Joback Method
dvisc	0.0008540	Pa×s	390.03	Joback Method
dvisc	0.0019703	Pa×s	351.81	Joback Method
dvisc	0.0055735	Pa×s	313.59	Joback Method
dvisc	0.0210426	Pa×s	275.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56009315&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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