Hexanoic acid, 3-hydroxy-, methyl ester

Other names:	Methyl 3-hydroxycaproate
	Methyl 3-hydroxyhexanoate
Inchi:	InChI=1S/C7H14O3/c1-3-4-6(8)5-7(9)10-2/h6,8H,3-5H2,1-2H3
InchiKey:	ACCRBMDJCPPJDX-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	CCCC(O)CC(=O)OC
Mol. weight [g/mol]:	146.18
CAS:	21188-58-9

Physical Properties

Property code	Value	Unit	Source
gf	-365.12	kJ/mol	Joback Method
hf	-590.12	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	56.62	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.710		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1049.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1031.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1626.00		NIST Webbook

ripol	1639.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1637.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1640.00		NIST Webbook
tb	527.59	K	Joback Method
tc	700.51	K	Joback Method
tf	286.63	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.76	J/mol×K	527.59	Joback Method
cpg	298.85	J/mol×K	556.41	Joback Method
cpg	308.56	J/mol×K	585.23	Joback Method
cpg	317.88	J/mol×K	614.05	Joback Method
cpg	326.83	J/mol×K	642.87	Joback Method
cpg	335.40	J/mol×K	671.69	Joback Method
cpg	343.59	J/mol×K	700.51	Joback Method
dvisc	0.0172601	Pa×s	286.63	Joback Method
dvisc	0.0045782	Pa×s	326.79	Joback Method
dvisc	0.0016237	Pa×s	366.95	Joback Method
dvisc	0.0007065	Pa×s	407.11	Joback Method
dvisc	0.0003570	Pa×s	447.27	Joback Method
dvisc	0.0002019	Pa×s	487.43	Joback Method
dvisc	0.0001245	Pa×s	527.59	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21188589&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume