Octanoic acid, 3-hydroxy-, methyl ester

Other names: methyl 3-hydroxyoctanoate
Inchi: InChI=1S/C9H18O3/c1-3-4-5-6-8(10)7-9(11)12-2/h8,10H,3-7H2,1-2H3
InchiKey: FHWBTAQRRDZDIY-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CCCCCC(O)CC(=O)OC
Mol. weight [g/mol]: 174.24
CAS: 7367-87-5

Physical Properties

Property code	Value	Unit	Source
gf	-348.28	kJ/mol	Joback Method
hf	-631.40	kJ/mol	Joback Method
hfus	22.42	kJ/mol	Joback Method
hvap	61.08	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.491		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1243.00		NIST Webbook
rinpol	1243.00		NIST Webbook
ripol	1850.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1835.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1850.00		NIST Webbook
tb	573.35	K	Joback Method
tc	743.84	K	Joback Method
tf	309.17	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.44	J/mol×K	573.35	Joback Method

cpg	392.26	J/mol×K	601.77	Joback Method
cpg	403.60	J/mol×K	630.18	Joback Method
cpg	414.48	J/mol×K	658.60	Joback Method
cpg	424.88	J/mol×K	687.01	Joback Method
cpg	434.83	J/mol×K	715.43	Joback Method
cpg	444.32	J/mol×K	743.84	Joback Method
dvisc	0.0115627	Pa×s	309.17	Joback Method
dvisc	0.0030766	Pa×s	353.20	Joback Method
dvisc	0.0010979	Pa×s	397.23	Joback Method
dvisc	0.0004812	Pa×s	441.26	Joback Method
dvisc	0.0002450	Pa×s	485.29	Joback Method
dvisc	0.0001395	Pa×s	529.32	Joback Method
dvisc	0.0000867	Pa×s	573.35	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7367875&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