Heptanoic acid, 3-hydroxy-, methyl ester

Other names:	Methyl 3-hydroxyheptanoate
	3-Hydroxy-heptanoic acid methyl ester
Inchi:	InChI=1S/C8H16O3/c1-3-4-5-7(9)6-8(10)11-2/h7,9H,3-6H2,1-2H3
InchiKey:	XSRWENVOBJMPPL-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCCCC(O)CC(=O)OC
Mol. weight [g/mol]:	160.21
CAS:	15889-95-9

Physical Properties

Property code	Value	Unit	Source
gf	-356.70	kJ/mol	Joback Method
hf	-610.76	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.101		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
tb	550.47	K	Joback Method
tc	722.09	K	Joback Method
tf	297.90	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.69	J/mol×K	550.47	Joback Method
cpg	344.69	J/mol×K	579.07	Joback Method
cpg	355.26	J/mol×K	607.68	Joback Method
cpg	365.40	J/mol×K	636.28	Joback Method

cpg	375.11	J/mol×K	664.88	Joback Method
cpg	384.41	J/mol×K	693.49	Joback Method
cpg	393.29	J/mol×K	722.09	Joback Method
dvisc	0.0141338	Pa×s	297.90	Joback Method
dvisc	0.0037547	Pa×s	340.00	Joback Method
dvisc	0.0013358	Pa×s	382.09	Joback Method
dvisc	0.0005834	Pa×s	424.19	Joback Method
dvisc	0.0002959	Pa×s	466.28	Joback Method
dvisc	0.0001680	Pa×s	508.38	Joback Method
dvisc	0.0001040	Pa×s	550.47	Joback Method

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=C15889959&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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