9-Hydroxy-decanoic acid, methyl ester

Other names: Methyl 9-hydroxydecanoate
Inchi: InChI=1S/C11H22O3/c1-10(12)8-6-4-3-5-7-9-11(13)14-2/h10,12H,3-9H2,1-2H3
InchiKey: RXJKTNNEUMHOQZ-UHFFFAOYSA-N
Formula: C11H22O3
SMILES: COC(=O)CCCCCCCC(C)O
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
gf	-331.44	kJ/mol	Joback Method
hf	-672.68	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.271		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2083.00		NIST Webbook
tb	619.11	K	Joback Method
tc	788.09	K	Joback Method
tf	331.71	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.00	J/mol×K	619.11	Joback Method
cpg	492.23	J/mol×K	647.27	Joback Method
cpg	504.91	J/mol×K	675.44	Joback Method
cpg	517.04	J/mol×K	703.60	Joback Method
cpg	528.63	J/mol×K	731.76	Joback Method

cpg	539.68	J/mol×K	759.93	Joback Method
cpg	550.21	J/mol×K	788.09	Joback Method
dvisc	0.0077301	Pa×s	331.71	Joback Method
dvisc	0.0020635	Pa×s	379.61	Joback Method
dvisc	0.0007406	Pa×s	427.51	Joback Method
dvisc	0.0003267	Pa×s	475.41	Joback Method
dvisc	0.0001675	Pa×s	523.31	Joback Method
dvisc	0.0000960	Pa×s	571.21	Joback Method
dvisc	0.0000600	Pa×s	619.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U194643&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

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