Methyl 3-hydroxydodecanoate

Other names: 3-Hydroxydodecanoic acid, methyl ester
Dodecanoic acid, 3-hydroxy, methyl ester
Inchi: InChI=1S/C13H26O3/c1-3-4-5-6-7-8-9-10-12(14)11-13(15)16-2/h12,14H,3-11H2,1-2H3
InchiKey: OZXCINYANGIBDB-UHFFFAOYSA-N
Formula: C13H26O3
SMILES: CCCCCCCCCC(O)CC(=O)OC
Mol. weight [g/mol]: 230.34
CAS: 72864-23-4

Physical Properties

Property code	Value	Unit	Source
gf	-314.60	kJ/mol	Joback Method
hf	-713.96	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	69.98	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.051		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
tb	664.87	K	Joback Method
tc	833.68	K	Joback Method
tf	354.25	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.63	J/mol×K	664.87	Joback Method
cpg	598.06	J/mol×K	693.00	Joback Method
cpg	611.86	J/mol×K	721.14	Joback Method
cpg	625.04	J/mol×K	749.27	Joback Method
cpg	637.60	J/mol×K	777.41	Joback Method

cpg	649.56	J/mol×K	805.54	Joback Method
cpg	660.93	J/mol×K	833.68	Joback Method
dvisc	0.0051687	Pa×s	354.25	Joback Method
dvisc	0.0013843	Pa×s	406.02	Joback Method
dvisc	0.0004994	Pa×s	457.79	Joback Method
dvisc	0.0002217	Pa×s	509.56	Joback Method
dvisc	0.0001143	Pa×s	561.33	Joback Method
dvisc	0.0000659	Pa×s	613.10	Joback Method
dvisc	0.0000414	Pa×s	664.87	Joback Method

Sources

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=C72864234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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