Methyl 10-hydroxyundecanoate

Inchi: InChI=1S/C12H24O3/c1-11(13)9-7-5-3-4-6-8-10-12(14)15-2/h11,13H,3-10H2,1-2H3
InchiKey: UFIVBIIQLDEBCZ-UHFFFAOYSA-N
Formula: C12H24O3
SMILES: COC(=O)CCCCCCCCCC(C)O
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
gf	-323.02	kJ/mol	Joback Method
hf	-693.32	kJ/mol	Joback Method
hfus	30.19	kJ/mol	Joback Method
hvap	67.75	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.661		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
ripol	2220.00		NIST Webbook
ripol	2220.00		NIST Webbook
tb	641.99	K	Joback Method
tc	810.69	K	Joback Method
tf	342.98	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.60	J/mol×K	641.99	Joback Method
cpg	594.01	J/mol×K	782.57	Joback Method
cpg	582.49	J/mol×K	754.46	Joback Method
cpg	570.39	J/mol×K	726.34	Joback Method
cpg	557.72	J/mol×K	698.22	Joback Method
cpg	544.46	J/mol×K	670.11	Joback Method

cpg	604.99	J/mol×K	810.69	Joback Method
dvisc	0.0000498	Pa×s	641.99	Joback Method
dvisc	0.0000796	Pa×s	592.15	Joback Method
dvisc	0.0001384	Pa×s	542.32	Joback Method
dvisc	0.0002691	Pa×s	492.49	Joback Method
dvisc	0.0006081	Pa×s	442.65	Joback Method
dvisc	0.0016900	Pa×s	392.81	Joback Method
dvisc	0.0063203	Pa×s	342.98	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R149527&Units=SI

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