Methyl 10-hydroxy-8-decenoate

Inchi: InChI=1S/C11H20O3/c1-14-11(13)9-7-5-3-2-4-6-8-10-12/h6,8,12H,2-5,7,9-10H2,1H3/b8-

InchiKey: YFYDEZMIUOGZLE-SOFGYWHQSA-N

Formula: C11H20O3

SMILES: COC(=O)CCCCCCC=CCO

Mol. weight [g/mol]: 200.27

Physical Properties

Property code	Value	Unit	Source
gf	-248.78	kJ/mol	Joback Method
hf	-550.18	kJ/mol	Joback Method
hfus	31.32	kJ/mol	Joback Method
hvap	65.87	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.048		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
ripol	2283.00		NIST Webbook
ripol	2283.00		NIST Webbook
tb	623.71	K	Joback Method
tc	795.65	K	Joback Method
tf	341.63	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.75	J/mol×K	623.71	Joback Method
cpg	470.25	J/mol×K	652.37	Joback Method
cpg	482.20	J/mol×K	681.02	Joback Method
cpg	493.61	J/mol×K	709.68	Joback Method
cpg	504.49	J/mol×K	738.34	Joback Method
cpg	514.87	J/mol×K	766.99	Joback Method

cpg	524.76	J/mol×K	795.65	Joback Method
dvisc	0.0049477	Pa×s	341.63	Joback Method
dvisc	0.0014790	Pa×s	388.64	Joback Method
dvisc	0.0005737	Pa×s	435.66	Joback Method
dvisc	0.0002677	Pa×s	482.67	Joback Method
dvisc	0.0001430	Pa×s	529.68	Joback Method
dvisc	0.0000846	Pa×s	576.70	Joback Method
dvisc	0.0000542	Pa×s	623.71	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R149498&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

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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