10-Hydroxydecanoic acid, methyl ester

Other names: Methyl 10-hydroxydecanoate
Inchi: InChI=1S/C11H22O3/c1-14-11(13)9-7-5-3-2-4-6-8-10-12/h12H,2-10H2,1H3
InchiKey: NFJQGHRDVMDLKM-UHFFFAOYSA-N
Formula: C11H22O3
SMILES: COC(=O)CCCCCCCCCO
Mol. weight [g/mol]: 202.29
CAS: 2640-94-0

Physical Properties

Property code	Value	Unit	Source
gf	-329.00	kJ/mol	Joback Method
hf	-667.40	kJ/mol	Joback Method
hfus	31.12	kJ/mol	Joback Method
hvap	65.92	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.273		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1567.00		NIST Webbook
rinpol	1567.00		NIST Webbook
ripol	2338.00		NIST Webbook
ripol	2338.00		NIST Webbook
tb	619.55	K	Joback Method
tc	786.12	K	Joback Method
tf	346.71	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.57	J/mol×K	619.55	Joback Method
cpg	491.58	J/mol×K	647.31	Joback Method
cpg	504.05	J/mol×K	675.07	Joback Method
cpg	515.99	J/mol×K	702.84	Joback Method

cpg	527.42	J/mol×K	730.60	Joback Method
cpg	538.33	J/mol×K	758.36	Joback Method
cpg	548.74	J/mol×K	786.12	Joback Method
dvisc	0.0050390	Pa×s	346.71	Joback Method
dvisc	0.0015980	Pa×s	392.18	Joback Method
dvisc	0.0006434	Pa×s	437.66	Joback Method
dvisc	0.0003074	Pa×s	483.13	Joback Method
dvisc	0.0001668	Pa×s	528.60	Joback Method
dvisc	0.0000997	Pa×s	574.08	Joback Method
dvisc	0.0000643	Pa×s	619.55	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=C2640940&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume