11-hydroxyundecanoic acid

Inchi: InChI=1S/C11H22O3/c12-10-8-6-4-2-1-3-5-7-9-11(13)14/h12H,1-10H2,(H,13,14)
InchiKey: KNRCBASNXNXUQQ-UHFFFAOYSA-N
Formula: C11H22O3
SMILES: O=C(O)CCCCCCCCCCO
Mol. weight [g/mol]: 202.29
CAS: 3669-80-5

Physical Properties

Property code	Value	Unit	Source
gf	-360.82	kJ/mol	Joback Method
hf	-687.41	kJ/mol	Joback Method
hfs	-920.00 ± 3.00	kJ/mol	NIST Webbook
hfus	34.02	kJ/mol	Joback Method
hvap	80.18	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.574		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
tb	689.31	K	Joback Method
tc	855.97	K	Joback Method
tf	385.30	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.66	J/mol×K	855.97	Joback Method
cpg	563.57	J/mol×K	828.20	Joback Method
cpg	554.02	J/mol×K	800.42	Joback Method
cpg	544.01	J/mol×K	772.64	Joback Method
cpg	533.51	J/mol×K	744.86	Joback Method
cpg	522.51	J/mol×K	717.09	Joback Method
cpg	510.99	J/mol×K	689.31	Joback Method
dvisc	0.0050547	Pa×s	385.30	Joback Method

dvisc	0.0000159	Pa×s	689.31	Joback Method
dvisc	0.0000284	Pa×s	638.64	Joback Method
dvisc	0.0000561	Pa×s	587.97	Joback Method
dvisc	0.0001257	Pa×s	537.30	Joback Method
dvisc	0.0003332	Pa×s	486.64	Joback Method
dvisc	0.0011081	Pa×s	435.97	Joback Method
hsubt	105.00	kJ/mol	314.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	0.50	NIST Webbook

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=C3669805&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
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume