Undecylenic acid

Other names:	10-Hendecenoic acid
	10-Henedecenoic acid
	10-Undecenoic acid
	10-Undecylenic acid
	Declid
	Desenex
	Desenex, solution
	Kyselina undecylenova
	NSC 2013
	Renselin
	Sevinon
	Undec-10-enoic acid
	Undecen-10-acid-1
	Undecenoic acid
	Undecyl-10-enic acid
	Undecylenenic acid
	n-Undecylenic acid
	undecylic acid
Inchi:	InChI=1S/C11H20O2/c1-2-3-4-5-6-7-8-9-10-11(12)13/h2H,1,3-10H2,(H,12,13)
InchiKey:	FRPZMMHWLSIFAZ-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	C=CCCCCCCCCC(=O)O
Mol. weight [g/mol]:	184.28
CAS:	112-38-9

Physical Properties

Property code	Value	Unit	Source
gf	-136.16	kJ/mol	Joback Method
hf	-409.75	kJ/mol	Joback Method
hfus	28.65	kJ/mol	Joback Method
hvap	62.83	kJ/mol	Joback Method
log10ws	-3.40		Aqueous Solubility Prediction Method
logp	3.378		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1484.30		NIST Webbook

rinpol	1484.30		NIST Webbook
rinpol	1421.00		NIST Webbook
ripol	2351.00		NIST Webbook
ripol	2358.00		NIST Webbook
tb	548.20	K	NIST Webbook
tc	762.49	K	Joback Method
tf	298.05 ± 1.00	K	NIST Webbook
tf	496.00 ± 2.00	K	NIST Webbook
tf	298.00 ± 0.50	K	NIST Webbook
tf	297.40	K	Aqueous Solubility Prediction Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.50	J/mol×K	762.49	Joback Method
cpg	488.53	J/mol×K	734.37	Joback Method
cpg	478.08	J/mol×K	706.26	Joback Method
cpg	467.13	J/mol×K	678.15	Joback Method
cpg	455.66	J/mol×K	650.04	Joback Method
cpg	443.64	J/mol×K	621.92	Joback Method
cpg	431.08	J/mol×K	593.81	Joback Method
dvisc	0.0090521	Pa×s	322.72	Joback Method
dvisc	0.0000916	Pa×s	593.81	Joback Method
dvisc	0.0001437	Pa×s	548.63	Joback Method
dvisc	0.0002445	Pa×s	503.45	Joback Method
dvisc	0.0004617	Pa×s	458.27	Joback Method
dvisc	0.0010022	Pa×s	413.08	Joback Method
dvisc	0.0026312	Pa×s	367.90	Joback Method
hvapt	70.60	kJ/mol	467.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	0.30	NIST Webbook
tbrp	410.00	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35239e+01
Coeff. B	-4.32806e+03
Coeff. C	-9.35360e+01
Temperature range (K), min.	420.52
Temperature range (K), max.	620.55

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112389&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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