Undecanoic acid

Other names:	1-Decanecarboxylic acid
	Hendecanoic acid
	Undecylic acid
	n-Undecanoic acid
	n-Undecoic acid
	n-Undecylic acid
	undedecanoic acid
Inchi:	InChI=1S/C11H22O2/c1-2-3-4-5-6-7-8-9-10-11(12)13/h2-10H2,1H3,(H,12,13)
InchiKey:	ZDPHROOEEOARMN-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	186.29
CAS:	112-37-8

Physical Properties

Property code	Value	Unit	Source
chl	-6736.50 ± 0.90	kJ/mol	NIST Webbook
gf	-224.00	kJ/mol	Joback Method
hf	-535.18	kJ/mol	Joback Method
hfus	29.93	kJ/mol	Joback Method
hsub	121.00 ± 1.00	kJ/mol	NIST Webbook
hsub	121.30 ± 1.30	kJ/mol	NIST Webbook
hvap	63.50	kJ/mol	Joback Method
log10ws	-3.55		Aqueous Solubility Prediction Method
logp	3.602		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2004.04 ± 90.00	kPa	NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	249.52		NIST Webbook

rinpol	248.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1466.80		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1468.00		NIST Webbook
ripol	2394.00		NIST Webbook
ripol	2401.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2413.00		NIST Webbook
ripol	2407.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2419.00		NIST Webbook
ripol	2417.00		NIST Webbook
ripol	2394.00		NIST Webbook
ripol	2398.00		NIST Webbook
ripol	2421.00		NIST Webbook
ripol	2419.00		NIST Webbook
ripol	2407.00		NIST Webbook
ripol	2405.00		NIST Webbook
ripol	2417.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2369.00		NIST Webbook
ripol	2379.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2371.00		NIST Webbook
ripol	2359.00		NIST Webbook
ripol	2400.00		NIST Webbook
tb	438.15	K	NIST Webbook
tb	553.15 ± 5.00	K	NIST Webbook
tc	731.26 ± 3.00	K	NIST Webbook
tf	301.65 ± 0.40	K	NIST Webbook
tf	302.00 ± 1.50	K	NIST Webbook
tf	301.20 ± 3.00	K	NIST Webbook
tf	301.58	K	Aqueous Solubility Prediction Method
tf	301.90 ± 0.05	K	NIST Webbook
tf	301.40 ± 0.20	K	NIST Webbook

tt	301.63 ± 0.02	K	NIST Webbook
tt	301.63	K	KDB
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.72	J/mol×K	763.46	Joback Method
cpg	501.22	J/mol×K	708.02	Joback Method
cpg	512.21	J/mol×K	735.74	Joback Method
cpg	452.00	J/mol×K	597.13	Joback Method
cpg	465.12	J/mol×K	624.85	Joback Method
cpg	477.69	J/mol×K	652.57	Joback Method
cpg	489.71	J/mol×K	680.30	Joback Method
cps	415.10	J/mol×K	293.00	NIST Webbook
cps	768.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0026360	Pa×s	369.92	Joback Method
dvisc	0.0004509	Pa×s	460.81	Joback Method
dvisc	0.0009898	Pa×s	415.36	Joback Method
dvisc	0.0000874	Pa×s	597.13	Joback Method
dvisc	0.0001380	Pa×s	551.69	Joback Method
dvisc	0.0002365	Pa×s	506.25	Joback Method
dvisc	0.0092362	Pa×s	324.48	Joback Method
hfust	25.98	kJ/mol	301.60	NIST Webbook
hfust	8.13	kJ/mol	290.00	NIST Webbook
hfust	25.98	kJ/mol	301.60	NIST Webbook
hvapt	97.90 ± 6.30	kJ/mol	305.50	NIST Webbook
hvapt	90.70 ± 2.00	kJ/mol	321.00	NIST Webbook
hvapt	81.30	kJ/mol	475.00	NIST Webbook
sfust	86.15	J/mol×K	301.60	NIST Webbook
sfust	28.03	J/mol×K	290.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	501.20	K	21.30	NIST Webbook
tbrp	437.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57164e+01
Coeff. B	-5.11747e+03
Coeff. C	-9.60380e+01
Temperature range (K), min.	427.72
Temperature range (K), max.	587.87

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.52629e+02
Coeff. B	-2.14898e+04
Coeff. C	-3.38776e+01
Coeff. D	1.53739e-05
Temperature range (K), min.	393.15
Temperature range (K), max.	557.15

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=945

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112378&Units=SI

Phase Equilibria of Long-Chain Carboxylic Acids in Supercritical Propane: https://www.doi.org/10.1021/je101077v

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=945

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume