N-TRIDECANOIC ACID

Other names:	N-TRIDECYLIC ACID
	Tridecanoic acid
	Tridecylic acid
	n-Tridecoic acid
Inchi:	InChI=1S/C13H26O2/c1-2-3-4-5-6-7-8-9-10-11-12-13(14)15/h2-12H2,1H3,(H,14,15)
InchiKey:	SZHOJFHSIKHZHA-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	214.35
CAS:	638-53-9

Physical Properties

Property code	Value	Unit	Source
af	0.9349		Cheméo Relay (1.0)
chl	-8024.20 ± 1.30	kJ/mol	NIST Webbook
gf	-207.16	kJ/mol	Joback Method
hf	-672.62	kJ/mol	Cheméo Relay (1.0)
hfus	35.11	kJ/mol	Joback Method
hsub	141.00	kJ/mol	NIST Webbook
hvap	103.01	kJ/mol	Cheméo Relay (1.0)
ie	9.94	eV	Cheméo Relay (1.0)
log10ws	-4.63		Cheméo Relay (1.0)
logp	4.382		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1748.88 ± 85.00	kPa	NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1667.20		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	278.19		NIST Webbook

rinpol	277.60		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1667.20		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1668.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2651.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2573.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2664.00		NIST Webbook
ripol	2573.00		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2570.00		NIST Webbook
tb	567.09	K	Cheméo Relay (1.0)
tc	754.01 ± 3.00	K	NIST Webbook
tf	313.70 ± 3.00	K	NIST Webbook
tf	314.65 ± 2.00	K	NIST Webbook
tf	315.10 ± 0.05	K	NIST Webbook
tf	314.95 ± 0.35	K	NIST Webbook
tt	315.01 ± 0.02	K	NIST Webbook
tt	315.01 ± 0.02	K	NIST Webbook
vc	0.776	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.04	J/mol×K	642.89	Joback Method
cpg	569.39	J/mol×K	670.56	Joback Method
cpg	583.12	J/mol×K	698.22	Joback Method
cpg	596.24	J/mol×K	725.89	Joback Method
cpg	608.78	J/mol×K	753.55	Joback Method
cpg	620.76	J/mol×K	781.22	Joback Method
cpg	632.19	J/mol×K	808.89	Joback Method
cps	387.60	J/mol×K	298.15	NIST Webbook

dvisc	0.0018042	Pa×s	396.33	Joback Method
dvisc	0.0006790	Pa×s	445.64	Joback Method
dvisc	0.0003105	Pa×s	494.95	Joback Method
dvisc	0.0001636	Pa×s	544.27	Joback Method
dvisc	0.0000959	Pa×s	593.58	Joback Method
dvisc	0.0000610	Pa×s	642.89	Joback Method
dvisc	0.0063287	Pa×s	347.02	Joback Method
hfust	8.72	kJ/mol	307.10	NIST Webbook
hfust	33.74	kJ/mol	315.00	NIST Webbook
hfust	33.74	kJ/mol	315.00	NIST Webbook
hfust	33.00	kJ/mol	314.60	NIST Webbook
hsubt	112.50	kJ/mol	276.50	NIST Webbook
hsubt	170.00	kJ/mol	290.50	NIST Webbook
hvapt	90.10	kJ/mol	497.00	NIST Webbook
hvapt	100.40 ± 2.00	kJ/mol	339.00	NIST Webbook
sfust	28.41	J/mol×K	307.10	NIST Webbook
sfust	107.11	J/mol×K	315.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	509.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61483e+01
Coeff. B	-5.49585e+03
Coeff. C	-1.03933e+02
Temperature range (K), min.	450.44
Temperature range (K), max.	611.08

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	4.05091e+02
Coeff. B	-3.06996e+04
Coeff. C	-5.59672e+01
Coeff. D	2.51191e-05
Temperature range (K), min.	409.15
Temperature range (K), max.	573.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=947
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638539&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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