Pentadecanoic acid

Other names:	Pentadecanoic (Palmitic) acid
	Pentadecylic acid
	n-Pentadecanoic acid
	n-Pentadecylic acid
Inchi:	InChI=1S/C15H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15(16)17/h2-14H2,1H3,(H,16,1
InchiKey:	WQEPLUUGTLDZJY-UHFFFAOYSA-N
Formula:	C15H30O2
SMILES:	CCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	242.40
CAS:	1002-84-2

Physical Properties

Property code	Value	Unit	Source
chl	-9327.70 ± 1.50	kJ/mol	NIST Webbook
gf	-190.32	kJ/mol	Joback Method
hf	-617.74	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hsub	156.00	kJ/mol	NIST Webbook
hvap	72.41	kJ/mol	Joback Method
log10ws	-4.31		Aqueous Solubility Prediction Method
logp	5.162		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1551.34 ± 85.00	kPa	NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1868.40		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1867.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1857.00		NIST Webbook

rinpol	1887.00	NIST Webbook
rinpol	1872.00	NIST Webbook
rinpol	1869.00	NIST Webbook
rinpol	1844.00	NIST Webbook
rinpol	1872.00	NIST Webbook
rinpol	1845.00	NIST Webbook
rinpol	1844.00	NIST Webbook
rinpol	1844.00	NIST Webbook
rinpol	1865.00	NIST Webbook
rinpol	1867.00	NIST Webbook
rinpol	1839.00	NIST Webbook
rinpol	1867.10	NIST Webbook
rinpol	1860.00	NIST Webbook
rinpol	1867.00	NIST Webbook
rinpol	1848.00	NIST Webbook
rinpol	1862.00	NIST Webbook
rinpol	1862.00	NIST Webbook
rinpol	1843.00	NIST Webbook
rinpol	1845.00	NIST Webbook
rinpol	1862.00	NIST Webbook
rinpol	1878.00	NIST Webbook
rinpol	1856.00	NIST Webbook
rinpol	1882.00	NIST Webbook
rinpol	1868.00	NIST Webbook
rinpol	1883.00	NIST Webbook
rinpol	1865.00	NIST Webbook
rinpol	1873.00	NIST Webbook
rinpol	1866.20	NIST Webbook
rinpol	1881.00	NIST Webbook
rinpol	1865.00	NIST Webbook
rinpol	1857.00	NIST Webbook
rinpol	1857.00	NIST Webbook
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rinpol	1870.00	NIST Webbook
rinpol	1880.00	NIST Webbook
rinpol	1858.00	NIST Webbook
rinpol	1866.00	NIST Webbook
rinpol	1868.00	NIST Webbook
rinpol	1858.00	NIST Webbook
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rinpol	1845.00	NIST Webbook
rinpol	1851.00	NIST Webbook
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rinpol	1877.00	NIST Webbook
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rinpol	1871.00	NIST Webbook
rinpol	1841.00	NIST Webbook
rinpol	1850.00	NIST Webbook
rinpol	1843.00	NIST Webbook
rinpol	308.82	NIST Webbook
rinpol	319.90	NIST Webbook
rinpol	306.30	NIST Webbook
rinpol	1877.00	NIST Webbook
rinpol	1873.00	NIST Webbook
rinpol	1865.00	NIST Webbook
rinpol	1855.00	NIST Webbook
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rinpol	1865.00	NIST Webbook
rinpol	1854.00	NIST Webbook
rinpol	1833.00	NIST Webbook
ripol	2791.00	NIST Webbook
ripol	2779.00	NIST Webbook
ripol	2791.00	NIST Webbook
ripol	2819.00	NIST Webbook
ripol	2821.00	NIST Webbook
ripol	2809.00	NIST Webbook
ripol	2819.00	NIST Webbook
ripol	2836.00	NIST Webbook
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ripol	2822.00		NIST Webbook
ripol	2805.00		NIST Webbook
ripol	2822.00		NIST Webbook
ripol	2822.00		NIST Webbook
ripol	2809.00		NIST Webbook
ripol	2822.00		NIST Webbook
ripol	2803.00		NIST Webbook
ripol	2822.00		NIST Webbook
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ripol	2822.00		NIST Webbook
ripol	2822.00		NIST Webbook
ripol	2822.00		NIST Webbook
ripol	2822.00		NIST Webbook
tb	688.65	K	Joback Method
tc	775.43 ± 3.00	K	NIST Webbook
tf	325.58	K	Aqueous Solubility Prediction Method
tt	325.68 ± 0.02	K	NIST Webbook
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.64	J/mol×K	688.65	Joback Method
cpg	679.08	J/mol×K	716.53	Joback Method
cpg	693.84	J/mol×K	744.41	Joback Method
cpg	707.94	J/mol×K	772.28	Joback Method
cpg	721.39	J/mol×K	800.16	Joback Method
cpg	734.21	J/mol×K	828.04	Joback Method
cpg	746.44	J/mol×K	855.92	Joback Method
cps	443.28	J/mol×K	298.15	NIST Webbook
dvisc	0.0012322	Pa×s	422.74	Joback Method
dvisc	0.0004648	Pa×s	475.92	Joback Method
dvisc	0.0002133	Pa×s	529.11	Joback Method
dvisc	0.0001128	Pa×s	582.29	Joback Method

dvisc	0.0000664	Pa×s	635.47	Joback Method
dvisc	0.0043252	Pa×s	369.56	Joback Method
dvisc	0.0000424	Pa×s	688.65	Joback Method
hfust	40.40	kJ/mol	325.50	NIST Webbook
hfust	41.52	kJ/mol	325.70	NIST Webbook
hfust	46.10	kJ/mol	324.90	NIST Webbook
hfust	8.12	kJ/mol	318.70	NIST Webbook
hfust	41.52	kJ/mol	325.70	NIST Webbook
hsubt	144.30	kJ/mol	284.00	NIST Webbook
hsubt	178.00	kJ/mol	294.00	NIST Webbook
hvapt	116.60	kJ/mol	298.00	Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of Some Fatty Acids
hvapt	94.00	kJ/mol	522.00	NIST Webbook
hvapt	108.50 ± 2.00	kJ/mol	357.00	NIST Webbook
sfust	127.49	J/mol×K	325.70	NIST Webbook
sfust	25.48	J/mol×K	318.70	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	530.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61706e+01
Coeff. B	-5.72495e+03
Coeff. C	-1.11355e+02
Temperature range (K), min.	471.80
Temperature range (K), max.	638.56

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.78309e+02
Coeff. B	-4.18615e+04
Coeff. C	-8.07117e+01
Coeff. D	3.36498e-05
Temperature range (K), min.	325.68
Temperature range (K), max.	766.40

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1002842&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=949
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=949
Vapor Pressures and Vaporization, Sublimation, and Fusion Enthalpies of some Fatty Acids:	https://www.doi.org/10.1021/je300902c
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hsubt:	Enthalpy of sublimation at a given temperature
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