Dotriacontane

Other names: BICETYL
n-Dotriacontane
Inchi: InChI=1S/C32H66/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-32-30-28-26-24-22-20-
InchiKey: QHMGJGNTMQDRQA-UHFFFAOYSA-N
Formula: C32H66
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 450.87
CAS: 544-85-4

Physical Properties

Property code	Value	Unit	Source
chs	-21056.80 ± 8.40	kJ/mol	NIST Webbook
gf	218.56	kJ/mol	Joback Method
hf	-696.60 ± 9.20	kJ/mol	NIST Webbook
hfs	-967.80 ± 8.80	kJ/mol	NIST Webbook
hfus	78.64	kJ/mol	Joback Method
hsub	271.20	kJ/mol	NIST Webbook
hsub	271.00 ± 3.00	kJ/mol	NIST Webbook
hvap	162.50	kJ/mol	NIST Webbook
log10ws	-13.22		Crippen Method
logp	12.729		Crippen Method
mcvol	461.740	ml/mol	McGowan Method
pc	543.36	kPa	Joback Method
rinpol	489.99		NIST Webbook
rinpol	489.99		NIST Webbook
ss	851.40	J/mol×K	NIST Webbook
tb	740.20	K	NIST Webbook
tc	342.80	K	KDB
tf	343.10 ± 0.40	K	NIST Webbook
tf	344.00 ± 2.00	K	NIST Webbook
tf	342.20 ± 1.00	K	NIST Webbook
tf	342.00 ± 4.00	K	NIST Webbook
tf	342.95 ± 0.60	K	NIST Webbook
tf	342.50 ± 0.50	K	NIST Webbook
tf	342.80 ± 0.30	K	NIST Webbook
tf	343.00 ± 0.30	K	NIST Webbook
tf	342.80 ± 1.00	K	NIST Webbook

tf	343.20 ± 0.50	K	NIST Webbook
tf	343.30 ± 0.50	K	NIST Webbook
tf	342.70 ± 2.00	K	NIST Webbook
tf	342.70 ± 1.00	K	NIST Webbook
tf	343.20 ± 1.00	K	NIST Webbook
tf	341.00 ± 2.00	K	NIST Webbook
tf	342.00 ± 4.00	K	NIST Webbook
tf	342.80 ± 0.50	K	NIST Webbook
tf	343.40 ± 1.00	K	NIST Webbook
tf	343.00 ± 2.00	K	NIST Webbook
tf	342.80 ± 1.50	K	NIST Webbook
tf	343.70 ± 1.00	K	NIST Webbook
tf	343.70 ± 1.00	K	NIST Webbook
tf	347.40 ± 4.00	K	NIST Webbook
tf	343.70 ± 1.00	K	NIST Webbook
tf	344.00 ± 6.00	K	NIST Webbook
tf	343.00 ± 1.00	K	NIST Webbook
tf	341.00 ± 5.00	K	NIST Webbook
tf	343.20 ± 3.00	K	NIST Webbook
tf	343.00 ± 2.00	K	NIST Webbook
tf	342.65 ± 0.50	K	NIST Webbook
tf	341.90 ± 2.00	K	NIST Webbook
tf	342.70 ± 1.00	K	NIST Webbook
tf	343.00 ± 2.00	K	NIST Webbook
tf	341.30 ± 2.00	K	NIST Webbook
tf	344.00 ± 2.00	K	NIST Webbook
tf	342.50 ± 0.50	K	NIST Webbook
tf	343.00 ± 2.00	K	NIST Webbook
tf	342.35 ± 0.50	K	NIST Webbook
tf	342.80	K	KDB
tf	342.37 ± 0.15	K	NIST Webbook
tt	338.10	K	Thermal conductivity of heavy, even-carbon number n-alkanes (C22 to C32)
vc	1.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1647.66	J/mol×K	969.38	Joback Method
cpg	1701.40	J/mol×K	1045.03	Joback Method

cpg	1675.39	J/mol×K	1007.21	Joback Method
cpg	1618.09	J/mol×K	931.56	Joback Method
cpg	1770.34	J/mol×K	1158.51	Joback Method
cpg	1748.76	J/mol×K	1120.68	Joback Method
cpg	1725.82	J/mol×K	1082.86	Joback Method
cpl	1356.00	J/mol×K	348.00	NIST Webbook
cps	1059.00	J/mol×K	338.00	NIST Webbook
cps	1038.00	J/mol×K	333.00	NIST Webbook
cps	877.40	J/mol×K	298.15	NIST Webbook
cps	806.00	J/mol×K	300.00	NIST Webbook
dvisc	0.0000179	Pa×s	931.56	Joback Method
dvisc	0.0000250	Pa×s	851.37	Joback Method
dvisc	0.0000376	Pa×s	771.17	Joback Method
dvisc	0.0000620	Pa×s	690.98	Joback Method
dvisc	0.0002652	Pa×s	530.59	Joback Method
dvisc	0.0008090	Pa×s	450.40	Joback Method
dvisc	0.0001165	Pa×s	610.79	Joback Method
hfust	76.57	kJ/mol	343.50	NIST Webbook
hfust	79.74	kJ/mol	341.90	NIST Webbook
hfust	41.38	kJ/mol	338.70	NIST Webbook
hfust	76.57	kJ/mol	343.50	NIST Webbook
hvapt	116.00	kJ/mol	625.50	NIST Webbook
hvapt	130.50	kJ/mol	378.00	NIST Webbook
hvapt	147.00 ± 1.00	kJ/mol	457.00	NIST Webbook
hvapt	162.50	kJ/mol	298.15	Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C31 to C38 at T = 298.15 K by Correlation Gas Chromatography
sfust	222.93	J/mol×K	343.50	NIST Webbook
sfust	122.18	J/mol×K	338.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53769e+01
Coeff. B	-6.36840e+03
Coeff. C	-1.46912e+02

Temperature range (K), min.	568.96
Temperature range (K), max.	779.61

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.93352e+02
Coeff. B	-3.72180e+04
Coeff. C	-5.24259e+01
Coeff. D	1.44473e-05
Temperature range (K), min.	510.15
Temperature range (K), max.	741.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C31 to C60 at T = 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je030236t
Experimental solubility data of various n-alkane waxes: effects of alkane chain length, alkane odd versus even carbon number structures, and solvent chemistry on solubility.	https://www.doi.org/10.1016/j.fluid.2004.10.021
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal conductivity of heavy, even-carbon number n-alkanes (C22 to C92):	https://www.doi.org/10.1016/j.fluid.2018.08.016
KDB:	https://www.cheric.org/files/research/kdb/mol/mol29.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C544854&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=29

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase 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
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume