Tritriacontane

Other names: n-Tritriacontane
Inchi: InChI=1S/C33H68/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-32-30-28-26-24-22-
InchiKey: SUJUOAZFECLBOA-UHFFFAOYSA-N
Formula: C33H68
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 464.89
CAS: 630-05-7

Physical Properties

Property code	Value	Unit	Source
gf	226.98	kJ/mol	Joback Method
hf	-724.45	kJ/mol	Joback Method
hfus	81.23	kJ/mol	Joback Method
hvap	167.60	kJ/mol	NIST Webbook
log10ws	-13.64		Crippen Method
logp	13.119		Crippen Method
mcvol	475.830	ml/mol	McGowan Method
pc	519.83	kPa	Joback Method
rinpol	500.99		NIST Webbook
ss	877.80	J/mol×K	NIST Webbook
tb	344.15	K	KDB
tc	1193.81	K	Joback Method
tf	345.20 ± 0.60	K	NIST Webbook
tf	344.30 ± 0.60	K	NIST Webbook
tf	344.30 ± 2.00	K	NIST Webbook
tf	344.30 ± 2.00	K	NIST Webbook
tf	342.60 ± 5.00	K	NIST Webbook
tf	345.00 ± 5.00	K	NIST Webbook
tf	345.00 ± 4.00	K	NIST Webbook
tf	345.00 ± 1.50	K	NIST Webbook
tf	350.00 ± 2.00	K	NIST Webbook
tf	344.20 ± 0.20	K	NIST Webbook
tf	344.70 ± 2.00	K	NIST Webbook
vc	1.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1844.59	J/mol×K	1193.81	Joback Method
cpg	1822.35	J/mol×K	1153.92	Joback Method
cpg	1798.68	J/mol×K	1114.02	Joback Method
cpg	1773.44	J/mol×K	1074.13	Joback Method
cpg	1746.46	J/mol×K	1034.23	Joback Method
cpg	1717.62	J/mol×K	994.34	Joback Method
cpg	1686.75	J/mol×K	954.44	Joback Method
cpl	1112.50	J/mol×K	353.00	NIST Webbook
cps	900.80	J/mol×K	294.40	NIST Webbook
dvisc	0.0000323	Pa×s	790.18	Joback Method
dvisc	0.0007002	Pa×s	461.67	Joback Method
dvisc	0.0000215	Pa×s	872.31	Joback Method
dvisc	0.0002289	Pa×s	543.80	Joback Method
dvisc	0.0001003	Pa×s	625.93	Joback Method
dvisc	0.0000533	Pa×s	708.05	Joback Method
dvisc	0.0000153	Pa×s	954.44	Joback Method
hfust	105.02	kJ/mol	344.00	NIST Webbook
hfust	105.04	kJ/mol	344.20	NIST Webbook
hvapt	118.00	kJ/mol	633.00	NIST Webbook
hvapt	148.00 ± 1.00	kJ/mol	459.00	NIST Webbook
hvapt	167.60	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	305.20	J/mol×K	344.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.29637e+01
Coeff. B	-1.78430e+04
Coeff. C	-6.66886e-04

Coeff. D	6.05571e-10
Temperature range (K), min.	434.15
Temperature range (K), max.	481.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=30
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol30.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C630057&Units=SI
Experimental solubility data of various n-alkane waxes: effects of alkane chain length, alkane odd versus even carbon number, structure, and solvent chemistry on solubility.	https://www.doi.org/10.1016/j.fluid.2004.10.021
Vapor Pressure and Vaporization Enthalpies of the n-Alkanes from C31 to C38 Measured by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je030236t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
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

vc: Critical Volume