Hentriacontane

Other names: Untriacontane
n-Hentriacontane
Inchi: InChI=1S/C31H64/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-30-28-26-24-22-20-18-
InchiKey: IUJAMGNYPWYUPM-UHFFFAOYSA-N
Formula: C31H64
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 436.84
CAS: 630-04-6

Physical Properties

Property code	Value	Unit	Source
gf	210.14	kJ/mol	Joback Method
hf	-683.17	kJ/mol	Joback Method
hfus	76.05	kJ/mol	Joback Method
hvap	157.30	kJ/mol	NIST Webbook
log10ws	-12.80		Crippen Method
logp	12.339		Crippen Method
mcvol	447.650	ml/mol	McGowan Method
pc	568.52	kPa	Joback Method
rinpol	472.70		NIST Webbook
rinpol	478.65		NIST Webbook
tb	908.68	K	Joback Method
tc	1124.59	K	Joback Method
tf	341.00 ± 1.00	K	NIST Webbook
tf	341.00 ± 2.00	K	NIST Webbook
tf	341.70 ± 1.00	K	NIST Webbook
tf	341.70 ± 1.00	K	NIST Webbook
tf	342.00 ± 2.00	K	NIST Webbook
tf	342.00 ± 2.00	K	NIST Webbook
tf	342.00 ± 2.00	K	NIST Webbook
tf	341.20 ± 4.00	K	NIST Webbook
tf	342.00 ± 2.00	K	NIST Webbook
tf	341.60 ± 4.00	K	NIST Webbook
tf	341.30 ± 3.00	K	NIST Webbook
tf	341.30 ± 5.00	K	NIST Webbook
tf	341.30 ± 3.00	K	NIST Webbook
tf	341.60 ± 0.60	K	NIST Webbook

tf	341.20 ± 0.60	K	NIST Webbook
tf	340.40 ± 0.10	K	NIST Webbook
tf	342.00 ± 1.00	K	NIST Webbook
tf	340.90 ± 0.50	K	NIST Webbook
vc	1.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1549.83	J/mol×K	908.68	Joback Method
cpg	1578.23	J/mol×K	944.67	Joback Method
cpg	1604.94	J/mol×K	980.65	Joback Method
cpg	1630.08	J/mol×K	1016.64	Joback Method
cpg	1653.73	J/mol×K	1052.62	Joback Method
cpg	1676.01	J/mol×K	1088.61	Joback Method
cpg	1697.00	J/mol×K	1124.59	Joback Method
cps	912.00	J/mol×K	323.00	NIST Webbook
dvisc	0.0003067	Pa×s	517.39	Joback Method
dvisc	0.0009328	Pa×s	439.13	Joback Method
dvisc	0.0001351	Pa×s	595.65	Joback Method
dvisc	0.0000720	Pa×s	673.90	Joback Method
dvisc	0.0000437	Pa×s	752.16	Joback Method
dvisc	0.0000292	Pa×s	830.42	Joback Method
dvisc	0.0000209	Pa×s	908.68	Joback Method
hvapt	157.30	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
hvapt	146.00 ± 2.00	kJ/mol	453.50	NIST Webbook
hvapt	113.80	kJ/mol	617.50	NIST Webbook

Correlations

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

Coeff. A	1.53473e+01
Coeff. B	-6.29509e+03
Coeff. C	-1.44410e+02
Temperature range (K), min.	562.42
Temperature range (K), max.	771.67

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures and Vaporization Enthalpies of the n-Alkanes from C31 to C38 at T = 298.15 K 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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C630046&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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