PENTATRIACONTANE

Other names: n-Pentatriacotane
n-pentatriacontane
Inchi: InChI=1S/C35H72/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-34-32-30-28-26-
InchiKey: VHQQPFLOGSTQPC-UHFFFAOYSA-N
Formula: C35H72
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 492.96

Physical Properties

Property code	Value	Unit	Source
af	1.3935		Cheméo Relay (1.0)
gf	243.82	kJ/mol	Joback Method
hf	-773.09	kJ/mol	Cheméo Relay (1.0)
hfus	86.41	kJ/mol	Joback Method
hvap	178.00	kJ/mol	NIST Webbook
ie	10.42	eV	Cheméo Relay (1.0)
log10ws	-12.75		Cheméo Relay (1.0)
logp	13.899		Crippen Method
mcvol	504.010	ml/mol	McGowan Method
pc	477.14	kPa	Joback Method
tb	763.20	K	NIST Webbook
tc	835.04	K	Cheméo Relay (1.0)
tf	349.00 ± 2.00	K	NIST Webbook
tf	347.00 ± 4.00	K	NIST Webbook
tf	347.70 ± 1.00	K	NIST Webbook
tf	347.20 ± 0.40	K	NIST Webbook
tf	347.70 ± 0.60	K	NIST Webbook
tf	347.80 ± 0.80	K	NIST Webbook
tf	347.00 ± 2.00	K	NIST Webbook
tf	346.00 ± 2.00	K	NIST Webbook
tf	346.00 ± 2.00	K	NIST Webbook
tf	346.00 ± 3.00	K	NIST Webbook
tf	349.00 ± 6.00	K	NIST Webbook
tf	347.90 ± 3.00	K	NIST Webbook
tf	347.90 ± 4.00	K	NIST Webbook
tf	347.90 ± 3.00	K	NIST Webbook
tf	347.90 ± 1.00	K	NIST Webbook

tf	347.70 ± 0.60	K	NIST Webbook
tf	347.60 ± 0.10	K	NIST Webbook
vc	2.036	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1825.17	J/mol×K	1000.20	Joback Method
cpg	1859.01	J/mol×K	1045.02	Joback Method
cpg	1890.41	J/mol×K	1089.84	Joback Method
cpg	1919.57	J/mol×K	1134.66	Joback Method
cpg	1946.73	J/mol×K	1179.47	Joback Method
cpg	1972.09	J/mol×K	1224.29	Joback Method
cpg	1995.88	J/mol×K	1269.11	Joback Method
cps	915.90	J/mol×K	302.00	NIST Webbook
dvisc	0.0000740	Pa×s	656.21	Joback Method
dvisc	0.0001695	Pa×s	570.21	Joback Method
dvisc	0.0005212	Pa×s	484.21	Joback Method
dvisc	0.0000392	Pa×s	742.20	Joback Method
dvisc	0.0000236	Pa×s	828.20	Joback Method
dvisc	0.0000157	Pa×s	914.20	Joback Method
dvisc	0.0000112	Pa×s	1000.20	Joback Method
hfust	86.40	kJ/mol	347.20	NIST Webbook
hfust	41.09	kJ/mol	344.70	NIST Webbook
hfust	86.40	kJ/mol	347.20	NIST Webbook
hvapt	178.00	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	122.40	kJ/mol	646.50	NIST Webbook
sfust	119.20	J/mol×K	344.70	NIST Webbook
sfust	248.85	J/mol×K	347.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	584.20	K	1.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C630079&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
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
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
vc:	Critical Volume

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