Tetratetracontane

Other names: n-Tetratetracontane
Inchi: InChI=1S/C44H90/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-44-
InchiKey: KMXFZRSJMDYPPG-UHFFFAOYSA-N
Formula: C44H90
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 619.19
CAS: 7098-22-8

Physical Properties

Property code	Value	Unit	Source
gf	319.60	kJ/mol	Joback Method
hf	-951.49	kJ/mol	Joback Method
hfus	109.72	kJ/mol	Joback Method
hvap	223.70 ± 0.90	kJ/mol	NIST Webbook
log10ws	-18.24		Crippen Method
logp	17.410		Crippen Method
mcvol	630.820	ml/mol	McGowan Method
pc	337.66	kPa	Joback Method
tb	1206.12	K	Joback Method
tc	919.00	K	Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique
tf	359.60 ± 2.00	K	NIST Webbook
tf	333.50 ± 2.00	K	NIST Webbook
tf	338.50 ± 1.50	K	NIST Webbook
tf	359.60 ± 2.00	K	NIST Webbook
tf	359.15 ± 0.50	K	NIST Webbook
vc	2.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2517.45	J/mol×K	1291.64	Joback Method

cpg	2568.54	J/mol×K	1377.16	Joback Method
cpg	2615.94	J/mol×K	1462.68	Joback Method
cpg	2755.16	J/mol×K	1719.23	Joback Method
cpg	2661.56	J/mol×K	1548.19	Joback Method
cpg	2707.32	J/mol×K	1633.71	Joback Method
cpg	2460.74	J/mol×K	1206.12	Joback Method
dvisc	0.0000036	Pa×s	1102.71	Joback Method
dvisc	0.0000055	Pa×s	999.29	Joback Method
dvisc	0.0000092	Pa×s	895.88	Joback Method
dvisc	0.0000176	Pa×s	792.47	Joback Method
dvisc	0.0000408	Pa×s	689.05	Joback Method
dvisc	0.0000026	Pa×s	1206.12	Joback Method
dvisc	0.0001278	Pa×s	585.64	Joback Method
hfust	145.50	kJ/mol	360.90	NIST Webbook
hfust	145.50	kJ/mol	360.90	NIST Webbook
hvapt	146.00	kJ/mol	387.00	NIST Webbook
hvapt	139.30	kJ/mol	699.00	NIST Webbook
hvapt	223.70	kJ/mol	298.15	Hypothetical Thermodynamic Properties: Vapor Pressures and Vaporization Enthalpies of the Even n-Alkanes from C40 to C76 at T = 298.15 K by Correlation-Gas Chromatography. Are the Vaporization Enthalpies a Linear Function of Carbon Number?

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39224e+01
Coeff. B	-5.44883e+03
Coeff. C	-2.46850e+02
Temperature range (K), min.	646.48
Temperature range (K), max.	879.63

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Critical temperatures and pressures of C40, C44, and C60 normal alkanes measured by the pulse-heating technique:	https://www.doi.org/10.1016/j.fluid.2014.07.017
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
Hypothetical Thermodynamic Properties: Vapor Pressures and Vaporization Enthalpies of the Even n-Alkanes from C40 to C76 at T = 298.15 K by Correlation-Gas Chromatography. Are the Vaporization Enthalpies a Linear Function of Carbon Number?:	https://www.doi.org/10.1021/je7005852
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7098228&Units=SI

Legend

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