Dotetracontane

Other names: n-Dotetracontane
Inchi: InChI=1S/C42H86/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-42-40-
InchiKey: FTJPDYTXORWVLU-UHFFFAOYSA-N
Formula: C42H86
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 591.13
CAS: 7098-20-6

Physical Properties

Property code	Value	Unit	Source
gf	302.76	kJ/mol	Joback Method
hf	-910.21	kJ/mol	Joback Method
hfus	165.97	kJ/mol	Observation of multiple phase transitions in some even n-alkanes using a high resolution and super-sensitive DSC
hvap	213.50	kJ/mol	NIST Webbook
log10ws	-17.40		Crippen Method
logp	16.630		Crippen Method
mcvol	602.640	ml/mol	McGowan Method
pc	362.81	kPa	Joback Method
tb	1160.36	K	Joback Method
tc	1598.77	K	Joback Method
tf	356.10 ± 2.00	K	NIST Webbook
tf	356.10 ± 4.00	K	NIST Webbook
vc	2.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2567.37	J/mol×K	1598.77	Joback Method
cpg	2530.29	J/mol×K	1525.70	Joback Method
cpg	2318.08	J/mol×K	1160.36	Joback Method
cpg	2367.91	J/mol×K	1233.43	Joback Method

cpg	2412.90	J/mol×K	1306.50	Joback Method
cpg	2454.20	J/mol×K	1379.56	Joback Method
cpg	2492.95	J/mol×K	1452.63	Joback Method
cpl	1425.00	J/mol×K	353.00	NIST Webbook
dvisc	0.0000050	Pa×s	1060.82	Joback Method
dvisc	0.0000036	Pa×s	1160.36	Joback Method
dvisc	0.0001763	Pa×s	563.10	Joback Method
dvisc	0.0000565	Pa×s	662.64	Joback Method
dvisc	0.0000244	Pa×s	762.19	Joback Method
dvisc	0.0000128	Pa×s	861.73	Joback Method
dvisc	0.0000076	Pa×s	961.27	Joback Method
hfust	165.97	kJ/mol	357.30	NIST Webbook
hvapt	136.00	kJ/mol	688.50	NIST Webbook
hvapt	213.50	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	1.41329e+01
Coeff. B	-5.48809e+03
Coeff. C	-2.40150e+02
Temperature range (K), min.	636.54
Temperature range (K), max.	862.28

Sources

Observation of multiple phase transitions in some even n-alkanes using a high resolution and super sensitive DSC:	https://www.doi.org/10.1016/j.tca.2006.06.022
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
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=C7098206&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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