

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:

FTJPDXORWVLU-UHFFFAOYSA-N

Formula:

C42H86

SMILES:

CC

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 ± 4.00	K	NIST Webbook
tf	356.10 ± 2.00	K	NIST Webbook
vc	2.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	2530.29	J/mol×K	1525.70	Joback Method
cpg	2567.37	J/mol×K	1598.77	Joback Method
cpl	1425.00	J/mol×K	353.00	NIST Webbook
dvisc	0.0000565	Paxs	662.64	Joback Method
dvisc	0.0001763	Paxs	563.10	Joback Method
dvisc	0.0000244	Paxs	762.19	Joback Method
dvisc	0.0000128	Paxs	861.73	Joback Method
dvisc	0.0000076	Paxs	961.27	Joback Method
dvisc	0.0000050	Paxs	1060.82	Joback Method
dvisc	0.0000036	Paxs	1160.36	Joback Method
hfust	165.97	kJ/mol	357.30	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?
hvapt	136.00	kJ/mol	688.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

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/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Observation of multiple phase transitions in some even n-alkanes

<https://www.doi.org/10.1016/j.tca.2006.06.022>

Hypothetical Thermodynamic Properties, Vapor Pressures and

<https://www.doi.org/10.1021/je7005852>

Vaporization Enthalpies of the Even

https://en.wikipedia.org/wiki/Joback_method

n-Alkanes from C₄₀ to C₇₆ at T =

<http://link.springer.com/article/10.1007/BF02311772>

McGowan Method:

Chromatography. Are the Vaporization Enthalpies a Linear Function of Carbon Number?:

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

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