n-Octatetracontane

Other names: octatetracontane
Inchi: InChI=1S/C48H98/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-45-
InchiKey: CFBPOLLJQOANPF-UHFFFAOYSA-N
Formula: C48H98
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 675.29
CAS: 7098-26-2

Physical Properties

Property code	Value	Unit	Source
gf	353.28	kJ/mol	Joback Method
hf	-1034.05	kJ/mol	Joback Method
hfus	120.08	kJ/mol	Joback Method
hvap	243.00 ± 0.20	kJ/mol	NIST Webbook
log10ws	-19.91		Crippen Method
logp	18.971		Crippen Method
mcvol	687.180	ml/mol	McGowan Method
pc	294.62	kPa	Joback Method
tb	1297.64	K	Joback Method
tc	2013.41	K	Joback Method
tf	361.40 ± 3.00	K	NIST Webbook
vc	2.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2748.26	J/mol×K	1297.64	Joback Method
cpg	2824.27	J/mol×K	1416.94	Joback Method
cpg	2894.38	J/mol×K	1536.23	Joback Method
cpg	2964.30	J/mol×K	1655.53	Joback Method
cpg	3039.75	J/mol×K	1774.82	Joback Method
cpg	3126.41	J/mol×K	1894.12	Joback Method
cpg	3230.01	J/mol×K	2013.41	Joback Method
cpl	1595.00	J/mol×K	353.00	NIST Webbook

dvisc	0.0000663	Pa×s	630.72	Joback Method
dvisc	0.0000211	Pa×s	741.87	Joback Method
dvisc	0.0000090	Pa×s	853.03	Joback Method
dvisc	0.0000047	Pa×s	964.18	Joback Method
dvisc	0.0000028	Pa×s	1075.33	Joback Method
dvisc	0.0000018	Pa×s	1186.49	Joback Method
dvisc	0.0000013	Pa×s	1297.64	Joback Method
hvapt	243.00	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	145.90	kJ/mol	719.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43954e+01
Coeff. B	-5.73112e+03
Coeff. C	-2.59450e+02
Temperature range (K), min.	665.69
Temperature range (K), max.	890.36

Sources

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
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=C7098262&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

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
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