

tetrahexacontane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C64H130/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-45

QEQOTIFAPIDGFL-UHFFFAOYSA-N

C64H130

CC

899.72

7719-87-1

Physical Properties

Property code	Value	Unit	Source
gf	488.00	kJ/mol	Joback Method
hf	-1364.29	kJ/mol	Joback Method
hfus	161.52	kJ/mol	Joback Method
hvap	315.40 ± 0.40	kJ/mol	NIST Webbook
log10ws	-26.61		Crippen Method
logp	25.212		Crippen Method
mcvol	912.620	ml/mol	McGowan Method
pc	184.51	kPa	Joback Method
tb	1663.72	K	Joback Method
tc	5509.01	K	Joback Method
tf	371.00 ± 4.00	K	NIST Webbook
tf	375.20 ± 0.25	K	NIST Webbook
tf	375.00 ± 4.00	K	NIST Webbook
vc	3.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3951.13	J/mol×K	1663.72	Joback Method
cpg	4785.54	J/mol×K	2304.60	Joback Method
cpg	7041.32	J/mol×K	2945.48	Joback Method
cpg	11903.65	J/mol×K	3586.36	Joback Method
cpg	20557.68	J/mol×K	4227.24	Joback Method
cpg	34188.57	J/mol×K	4868.13	Joback Method
cpg	53981.47	J/mol×K	5509.01	Joback Method

dvisc	0.0000013	Pa×s	953.15	Joback Method
dvisc	0.0000043	Pa×s	811.04	Joback Method
dvisc	0.0000006	Pa×s	1095.27	Joback Method
dvisc	0.0000003	Pa×s	1237.38	Joback Method
dvisc	0.0000002	Pa×s	1379.49	Joback Method
dvisc	0.0000001	Pa×s	1521.61	Joback Method
dvisc	7.7953927e-08	Pa×s	1663.72	Joback Method
hvapt	315.40	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	168.30	kJ/mol	778.50	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7719871&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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>

Legend

cp _g :	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g _f :	Standard Gibbs free energy of formation
h _f :	Enthalpy of formation at standard conditions
h _{fus} :	Enthalpy of fusion at standard conditions
h _{vap} :	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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