N-heptadecylcyclohexane

Other names: Cyclohexane, heptadecyl-
Heptadecylcyclohexane
Hexadecylcyclohexane
Inchi: InChI=1S/C23H46/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23-21-18-16-19-22-23/h2
InchiKey: VLHZQNGNJQYAIZ-UHFFFAOYSA-N
Formula: C23H46
SMILES: CCCCCCCCCCCCCCCCCCC1CCCCC1
Mol. weight [g/mol]: 322.62
CAS: 19781-73-8

Physical Properties

Property code	Value	Unit	Source
af	0.8538		Cheméo Relay (1.0)
gf	167.23	kJ/mol	Joback Method
hf	-474.01	kJ/mol	Cheméo Relay (1.0)
hfus	47.16	kJ/mol	Joback Method
hvap	112.96	kJ/mol	Cheméo Relay (1.0)
ie	9.98	eV	Cheméo Relay (1.0)
log10ws	-9.22		Cheméo Relay (1.0)
logp	8.828		Crippen Method
mcvol	324.070	ml/mol	McGowan Method
pc	963.87	kPa	Joback Method
rinpol	372.80		NIST Webbook
tb	629.31	K	Cheméo Relay (1.0)
tc	807.66	K	Cheméo Relay (1.0)
tf	299.72	K	Cheméo Relay (1.0)
vc	1.247	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.43	J/mol×K	894.63	Joback Method
cpg	1149.55	J/mol×K	924.52	Joback Method
cpg	1048.20	J/mol×K	775.08	Joback Method

cpg	1070.71	J/mol×K	804.97	Joback Method
cpg	1092.06	J/mol×K	834.85	Joback Method
cpg	1112.28	J/mol×K	864.74	Joback Method
cpg	1024.48	J/mol×K	745.19	Joback Method
dvisc	0.0004454	Pa×s	485.96	Joback Method
dvisc	0.0010147	Pa×s	421.16	Joback Method
dvisc	0.0031190	Pa×s	356.35	Joback Method
dvisc	0.0002373	Pa×s	550.77	Joback Method
dvisc	0.0001444	Pa×s	615.58	Joback Method
dvisc	0.0000965	Pa×s	680.38	Joback Method
dvisc	0.0000692	Pa×s	745.19	Joback Method
hvapt	97.60	kJ/mol	539.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49287e+01
Coeff. B	-5.04154e+03
Coeff. C	-1.60369e+02
Temperature range (K), min.	504.71
Temperature range (K), max.	684.59

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781738&Units=SI

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume