TETRADECYLCYCLOHEXANE

Other names:	cyclohexane, tetradecyl- n-Tetradecylcyclohexane n-tetradecycyclohexane tetradecane, 1-cyclohexyl-
Inchi:	InChI=1S/C20H40/c1-2-3-4-5-6-7-8-9-10-11-12-14-17-20-18-15-13-16-19-20/h20H,2-19H
InchiKey:	NQAVPKIJZCHUNS-UHFFFAOYSA-N
Formula:	C20H40
SMILES:	CCCCCCCCCCCCCCC1CCCCC1
Mol. weight [g/mol]:	280.54
CAS:	1795-18-2

Physical Properties

Property code	Value	Unit	Source
af	0.7482		Cheméo Relay (1.0)
chl	-13167.80 ± 3.00	kJ/mol	NIST Webbook
gf	141.97	kJ/mol	Joback Method
hf	-419.30 ± 3.30	kJ/mol	NIST Webbook
hfus	39.39	kJ/mol	Joback Method
hvap	99.40	kJ/mol	NIST Webbook
ie	9.88	eV	Cheméo Relay (1.0)
log10ws	-8.40		Cheméo Relay (1.0)
logp	7.658		Crippen Method
mcvol	281.800	ml/mol	McGowan Method
pc	1162.45	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2079.10		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2016.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2084.70		NIST Webbook
ripol	2106.00		NIST Webbook
ripol	2106.00		NIST Webbook
tb	611.00 ± 4.00	K	NIST Webbook
tc	785.43	K	Cheméo Relay (1.0)

tf	298.00 ± 1.50	K	NIST Webbook
vc	1.076	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.76	J/mol×K	676.55	Joback Method
cpg	862.04	J/mol×K	706.33	Joback Method
cpg	884.17	J/mol×K	736.12	Joback Method
cpg	905.19	J/mol×K	765.90	Joback Method
cpg	925.15	J/mol×K	795.69	Joback Method
cpg	944.07	J/mol×K	825.47	Joback Method
cpg	962.00	J/mol×K	855.26	Joback Method
dvisc	0.0044101	Pa×s	322.54	Joback Method
dvisc	0.0014515	Pa×s	381.54	Joback Method
dvisc	0.0006434	Pa×s	440.54	Joback Method
dvisc	0.0003456	Pa×s	499.54	Joback Method
dvisc	0.0002117	Pa×s	558.55	Joback Method
dvisc	0.0001424	Pa×s	617.55	Joback Method
dvisc	0.0001026	Pa×s	676.55	Joback Method
hvapt	74.70	kJ/mol	575.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	297.20	K	100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	302.20	K	20000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	307.00	K	39900.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes

tfp	311.50	K	60000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	316.00	K	79900.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	320.30	K	100100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54021e+01
Coeff. B	-5.09371e+03
Coeff. C	-1.38651e+02
Temperature range (K), min.	475.66
Temperature range (K), max.	643.45

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

KDB: https://www.cheric.org/files/research/kdb/mol/mol605.mol

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795182&Units=SI

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

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

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

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

Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes: https://www.doi.org/10.1021/je600575r

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

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
vc:	Critical Volume