Cyclopentane, tetradecyl-

Other names: TETRADECYLCYCLOPENTANE
n-Tetradecylcyclopentane
Inchi: InChI=1S/C19H38/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-19-17-14-15-18-19/h19H,2-18H2,1
InchiKey: MJWRHKSSZBHAEW-UHFFFAOYSA-N
Formula: C19H38
SMILES: CCCCCCCCCCCCCCC1CCCC1
Mol. weight [g/mol]: 266.50
CAS: 1795-22-8

Physical Properties

Property code	Value	Unit	Source
af	0.7890		KDB
chl	-12533.30 ± 2.90	kJ/mol	NIST Webbook
gf	145.60	kJ/mol	KDB
hf	-374.40 ± 3.10	kJ/mol	NIST Webbook
hf	-374.60	kJ/mol	KDB
hfus	38.90	kJ/mol	Joback Method
hvap	95.40	kJ/mol	NIST Webbook
log10ws	-7.43		Crippen Method
logp	7.268		Crippen Method
mcvol	267.710	ml/mol	McGowan Method
pc	1120.00	kPa	KDB
rinpol	1974.00		NIST Webbook
rinpol	1975.40		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1966.80		NIST Webbook
ripol	1986.70		NIST Webbook
ripol	1986.70		NIST Webbook
tb	599.00	K	KDB
tc	772.00	K	KDB
tf	282.00	K	KDB
tf	281.00 ± 1.50	K	NIST Webbook
tf	281.20 ± 1.00	K	NIST Webbook
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.40	J/mol×K	649.40	Joback Method
cpg	797.76	J/mol×K	678.56	Joback Method
cpg	819.08	J/mol×K	707.73	Joback Method
cpg	839.37	J/mol×K	736.89	Joback Method
cpg	858.69	J/mol×K	766.06	Joback Method
cpg	877.07	J/mol×K	795.22	Joback Method
cpg	894.55	J/mol×K	824.39	Joback Method
dvisc	0.0007864	Pa×s	426.33	Joback Method
dvisc	0.0015991	Pa×s	370.56	Joback Method
dvisc	0.0041812	Pa×s	314.79	Joback Method
dvisc	0.0004558	Pa×s	482.09	Joback Method
dvisc	0.0002958	Pa×s	537.86	Joback Method
dvisc	0.0002082	Pa×s	593.63	Joback Method
dvisc	0.0001557	Pa×s	649.40	Joback Method
hvapt	55.98	kJ/mol	612.20	KDB
hvapt	73.60	kJ/mol	561.50	NIST Webbook
rhol	820.00	kg/m3	293.00	KDB
srf	0.02	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.90996e+02
Coeff. B	-1.87978e+04
Coeff. C	-2.46912e+01
Coeff. D	8.10603e-06
Temperature range (K), min.	465.00
Temperature range (K), max.	648.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol602.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795228&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=602
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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