n-Pentadecylcyclopentane

Other names: Pentadecylcyclopentane
Inchi: InChI=1S/C20H40/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-18-15-16-19-20/h20H,2-19H
InchiKey: HENJCAULAAJZLZ-UHFFFAOYSA-N
Formula: C20H40
SMILES: CCCCCCCCCCCCCCCC1CCCC1
Mol. weight [g/mol]: 280.53
CAS: 4669-01-6

Physical Properties

Property code	Value	Unit	Source
af	0.8330		KDB
gf	154.00	kJ/mol	KDB
hf	-395.30	kJ/mol	KDB
hfus	41.49	kJ/mol	Joback Method
hvap	100.30	kJ/mol	NIST Webbook
log10ws	-7.85		Crippen Method
logp	7.658		Crippen Method
mcvol	281.800	ml/mol	McGowan Method
pc	1020.00	kPa	KDB
rinpol	2068.00		NIST Webbook
tb	625.00	K	KDB
tc	780.00	K	KDB
tf	290.00	K	KDB
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.57	J/mol×K	759.58	Joback Method
cpg	955.19	J/mol×K	846.89	Joback Method
cpg	937.58	J/mol×K	817.79	Joback Method
cpg	919.05	J/mol×K	788.69	Joback Method
cpg	835.02	J/mol×K	672.28	Joback Method
cpg	857.59	J/mol×K	701.38	Joback Method

cpg	879.09	J/mol×K	730.48	Joback Method
dvisc	0.0001390	Pa×s	672.28	Joback Method
dvisc	0.0004117	Pa×s	499.17	Joback Method
dvisc	0.0002660	Pa×s	556.87	Joback Method
dvisc	0.0001865	Pa×s	614.58	Joback Method
dvisc	0.0038610	Pa×s	326.06	Joback Method
dvisc	0.0014629	Pa×s	383.76	Joback Method
dvisc	0.0007144	Pa×s	441.47	Joback Method
hvapt	76.50	kJ/mol	573.50	NIST Webbook
hvapt	57.66	kJ/mol	625.00	KDB
rhol	821.00	kg/m3	293.00	KDB
srf	0.02	N/m	323.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59948e+01
Coeff. B	-5.64829e+03
Coeff. C	-1.14900e+02
Temperature range (K), min.	474.50
Temperature range (K), max.	643.60

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/mol604.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4669016&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

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
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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume