

Tridecylcyclopentane

Other names:	n-Tridecylcyclopentane
Inchi:	InChI=1S/C18H36/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-16-13-14-17-18/h18H,2-17H2,1H3
InchiKey:	NYZHNJGPFXXHNR-UHFFFAOYSA-N
Formula:	C18H36
SMILES:	CCCCCCCCCCCCCCC1CCCC1
Mol. weight [g/mol]:	252.48
CAS:	6006-34-4

Physical Properties

Property code	Value	Unit	Source
af	0.6970		KDB
chl	-11874.60 ± 2.70	kJ/mol	NIST Webbook
gf	137.10	kJ/mol	KDB
hf	-353.80 ± 2.90	kJ/mol	NIST Webbook
hf	-354.00	kJ/mol	KDB
hfus	36.31	kJ/mol	Joback Method
hvap	90.50	kJ/mol	NIST Webbook
log10ws	-7.01		Crippen Method
logp	6.878		Crippen Method
mcvol	253.620	ml/mol	McGowan Method
pc	1310.00	kPa	KDB
rinpol	1862.00		NIST Webbook
tb	598.60	K	KDB
tc	766.50	K	KDB
tf	278.00	K	KDB
vc	0.985	m ³ /kmol	KDB
zc	0.2023660		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.94	J/mol×K	802.27	Joback Method
cpg	716.91	J/mol×K	626.52	Joback Method
cpg	739.05	J/mol×K	655.81	Joback Method

cpg	760.16	J/molxK	685.10	Joback Method
cpg	780.27	J/molxK	714.40	Joback Method
cpg	799.41	J/molxK	743.69	Joback Method
cpg	817.62	J/molxK	772.98	Joback Method
dvisc	0.0001734	Paxs	626.52	Joback Method
dvisc	0.0044926	Paxs	303.52	Joback Method
dvisc	0.0017356	Paxs	357.35	Joback Method
dvisc	0.0008601	Paxs	411.19	Joback Method
dvisc	0.0005015	Paxs	465.02	Joback Method
dvisc	0.0003270	Paxs	518.85	Joback Method
dvisc	0.0002311	Paxs	572.69	Joback Method
hvapt	70.90	kJ/mol	548.50	NIST Webbook
hvapt	54.31	kJ/mol	598.60	KDB
rhol	818.00	kg/m3	293.00	KDB
srf	0.03	N/m	298.20	KDB

Sources

The Yaws Handbook of Vapor Pressure:
KDB Vapor Pressure Data:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=600>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

https://www.chemo.com/doc/models/crippen_log10ws

KDB:

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

McGowan Method:

<https://www.thermo.com/files/research/kdb/mol/mol600.mol>

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6006344&Units=SI>

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
rhol:	Liquid Density
rinpola:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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