Cyclopentane, heptyl-

Other names:	1-CYCLOPENTYLHEPTANE
	HEPTYLCYCLOPENTANE
	n-Heptylcyclopentane
Inchi:	InChI=1S/C12H24/c1-2-3-4-5-6-9-12-10-7-8-11-12/h12H,2-11H2,1H3
InchiKey:	BOFNAOHMSHEKQL-UHFFFAOYSA-N
Formula:	C12H24
SMILES:	CCCCCCCC1CCCC1
Mol. weight [g/mol]:	168.32
CAS:	5617-42-5

Physical Properties

Property code	Value	Unit	Source
af	0.5150		KDB
chl	-7922.10 ± 1.60	kJ/mol	NIST Webbook
gf	86.67	kJ/mol	KDB
hf	-230.30	kJ/mol	KDB
hf	-230.10 ± 1.80	kJ/mol	NIST Webbook
hfus	20.77	kJ/mol	Joback Method
hvap	60.80	kJ/mol	NIST Webbook
log10ws	-4.50		Crippen Method
logp	4.537		Crippen Method
mcvol	169.080	ml/mol	McGowan Method
pc	1940.00	kPa	KDB
rinpol	1234.00		NIST Webbook
ripol	1304.90		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1303.00		NIST Webbook
tb	497.07 ± 0.50	K	NIST Webbook
tb	497.07 ± 0.20	K	NIST Webbook
tb	497.30	K	KDB
tc	679.00	K	KDB
tf	212.11 ± 0.50	K	NIST Webbook
tf	212.11 ± 0.20	K	NIST Webbook
tf	220.00	K	KDB
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.31	J/mol×K	674.70	Joback Method
cpg	394.52	J/mol×K	489.24	Joback Method
cpg	414.39	J/mol×K	520.15	Joback Method
cpg	433.32	J/mol×K	551.06	Joback Method
cpg	451.35	J/mol×K	581.97	Joback Method
cpg	468.51	J/mol×K	612.88	Joback Method
cpg	484.82	J/mol×K	643.79	Joback Method
dvisc	0.0002835	Pa×s	489.24	Joback Method
dvisc	0.0055055	Pa×s	235.90	Joback Method
dvisc	0.0023074	Pa×s	278.12	Joback Method
dvisc	0.0012162	Pa×s	320.35	Joback Method
dvisc	0.0007442	Pa×s	362.57	Joback Method
dvisc	0.0005045	Pa×s	404.79	Joback Method
dvisc	0.0003681	Pa×s	447.02	Joback Method
hvapt	43.35	kJ/mol	497.30	KDB
rhol	810.00	kg/m3	293.00	KDB
srf	0.03	N/m	298.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47895e+01
Coeff. B	-4.24819e+03
Coeff. C	-7.93990e+01
Temperature range (K), min.	372.34
Temperature range (K), max.	527.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.21686e+02

Coeff. B	-1.16261e+04
Coeff. C	-1.53646e+01
Coeff. D	6.91950e-06
Temperature range (K), min.	368.00
Temperature range (K), max.	679.00

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/mol593.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5617425&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=593
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