1,5-Cyclooctadiene

Other names: CYCLOOCTA-1,5-DIENE
Inchi: InChI=1S/C8H12/c1-2-4-6-8-7-5-3-1/h1-2,7-8H,3-6H2
InchiKey: VYXHVRARDIDEHS-UHFFFAOYSA-N
Formula: C8H12
SMILES: C1=CCCC=CCC1
Mol. weight [g/mol]: 108.18
CAS: 111-78-4

Physical Properties

Property code	Value	Unit	Source
chl	-4887.00 ± 3.00	kJ/mol	NIST Webbook
gf	84.36	kJ/mol	Joback Method
hf	57.00 ± 3.00	kJ/mol	NIST Webbook
hfl	24.00 ± 3.00	kJ/mol	NIST Webbook
hfus	5.48	kJ/mol	Joback Method
hvap	33.00	kJ/mol	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.673		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	923.00		NIST Webbook
rinpol	923.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1164.00		NIST Webbook
sl	264.30	J/mol×K	NIST Webbook
sl	250.00	J/mol×K	NIST Webbook
tb	422.00 ± 3.00	K	NIST Webbook
tb	422.70	K	NIST Webbook
tc	637.21	K	Joback Method
tf	204.00 ± 4.00	K	NIST Webbook
tf	201.00 ± 4.00	K	NIST Webbook
tf	203.80 ± 0.06	K	NIST Webbook
tt	203.98 ± 0.02	K	NIST Webbook
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.98	J/mol×K	637.21	Joback Method
cpg	183.96	J/mol×K	413.52	Joback Method
cpg	258.65	J/mol×K	599.93	Joback Method
cpg	245.48	J/mol×K	562.65	Joback Method
cpg	231.45	J/mol×K	525.37	Joback Method
cpg	216.53	J/mol×K	488.08	Joback Method
cpg	200.71	J/mol×K	450.80	Joback Method
cpl	208.10	J/mol×K	298.15	NIST Webbook
cpl	198.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0002081	Pa×s	413.52	Joback Method
dvisc	0.0063666	Pa×s	223.94	Joback Method
dvisc	0.0291355	Pa×s	186.02	Joback Method
dvisc	0.0003129	Pa×s	375.60	Joback Method
dvisc	0.0005156	Pa×s	337.69	Joback Method
dvisc	0.0009642	Pa×s	299.77	Joback Method
dvisc	0.0021612	Pa×s	261.85	Joback Method
hfust	9.83	kJ/mol	204.00	NIST Webbook
hfust	-0.38	kJ/mol	194.40	NIST Webbook
sfust	48.20	J/mol×K	194.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44781e+01
Coeff. B	-3.68378e+03
Coeff. C	-4.90830e+01
Temperature range (K), min.	308.68
Temperature range (K), max.	450.95

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.11397e+01
Coeff. B	-7.59295e+03
Coeff. C	-8.15275e+00
Coeff. D	3.91389e-06
Temperature range (K), min.	203.98
Temperature range (K), max.	645.00

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=634
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111784&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=634
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume