Cyclooctene

Other names: (Z)-Cyclooctene
Inchi: InChI=1S/C8H14/c1-2-4-6-8-7-5-3-1/h1-2H,3-8H2
InchiKey: URYYVOIYTNXXBN-UHFFFAOYSA-N
Formula: C8H14
SMILES: C1=CCCCCCC1
Mol. weight [g/mol]: 110.20
CAS: 931-88-4

Physical Properties

Property code	Value	Unit	Source
gf	54.40	kJ/mol	Joback Method
hf	-88.33	kJ/mol	Joback Method
hfus	4.26	kJ/mol	Joback Method
hvap	34.78	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
log10ws	-2.92		Crippen Method
logp	2.897		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
rinpol	892.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	899.00		NIST Webbook

rinpol	945.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	900.00		NIST Webbook
ripol	1035.00		NIST Webbook
ripol	955.00		NIST Webbook
sl	254.50	J/mol×K	NIST Webbook
tb	414.36	K	Joback Method
tc	635.63	K	Joback Method
tf	185.26	K	Joback Method
tt	259.15 ± 0.02	K	NIST Webbook
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.12	J/mol×K	561.87	Joback Method
cpg	248.81	J/mol×K	524.99	Joback Method
cpg	292.07	J/mol×K	635.63	Joback Method
cpg	278.54	J/mol×K	598.75	Joback Method
cpg	197.28	J/mol×K	414.36	Joback Method
cpg	215.41	J/mol×K	451.24	Joback Method
cpg	232.58	J/mol×K	488.12	Joback Method
cpl	207.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0011148	Pa×s	299.81	Joback Method
dvisc	0.0002186	Pa×s	414.36	Joback Method
dvisc	0.0005729	Pa×s	337.99	Joback Method
dvisc	0.0003370	Pa×s	376.18	Joback Method
dvisc	0.0426132	Pa×s	185.26	Joback Method
dvisc	0.0083526	Pa×s	223.44	Joback Method
dvisc	0.0026344	Pa×s	261.63	Joback Method
hfust	1.81	kJ/mol	259.20	NIST Webbook
hfust	1.81	kJ/mol	259.20	NIST Webbook
hfust	9.80	kJ/mol	190.10	NIST Webbook
hvapt	41.60	kJ/mol	303.00	NIST Webbook
hvapt	42.00	kJ/mol	342.00	NIST Webbook
sfust	6.98	J/mol×K	259.20	NIST Webbook
sfust	51.55	J/mol×K	190.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61864e+01
Coeff. B	-4.62219e+03
Coeff. C	-1.51380e+01
Temperature range (K), min.	273.00
Temperature range (K), max.	440.17

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C931884&Units=SI

Legend

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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