1,3-Cyclooctadiene

Other names: cycloocta-1,3-diene
Inchi: InChI=1S/C8H12/c1-2-4-6-8-7-5-3-1/h1-4H,5-8H2/b3-1-,4-2?
InchiKey: RRKODOZNUZCUBN-PBIXIIOPSA-N
Formula: C8H12
SMILES: C1=CCCCCC=C1
Mol. weight [g/mol]: 108.18
CAS: 1700-10-3

Physical Properties

Property code	Value	Unit	Source
gf	84.36	kJ/mol	Joback Method
hf	-30.55	kJ/mol	Joback Method
hfus	5.48	kJ/mol	Joback Method
hvap	35.07	kJ/mol	Joback Method
ie	8.40	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	894.00		NIST Webbook
rinpol	894.00		NIST Webbook
ripol	1100.00		NIST Webbook
tb	413.52	K	Joback Method
tc	637.21	K	Joback Method
tf	186.02	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.96	J/mol×K	413.52	Joback Method
cpg	200.71	J/mol×K	450.80	Joback Method
cpg	216.53	J/mol×K	488.08	Joback Method
cpg	231.45	J/mol×K	525.37	Joback Method

cpg	245.48	J/mol×K	562.65	Joback Method
cpg	258.65	J/mol×K	599.93	Joback Method
cpg	270.98	J/mol×K	637.21	Joback Method
dvisc	0.0291355	Pa×s	186.02	Joback Method
dvisc	0.0063666	Pa×s	223.94	Joback Method
dvisc	0.0021612	Pa×s	261.85	Joback Method
dvisc	0.0009642	Pa×s	299.77	Joback Method
dvisc	0.0005156	Pa×s	337.69	Joback Method
dvisc	0.0003129	Pa×s	375.60	Joback Method
dvisc	0.0002081	Pa×s	413.52	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36434e+01
Coeff. B	-3.28660e+03
Coeff. C	-5.68400e+01
Temperature range (K), min.	302.92
Temperature range (K), max.	451.30

Sources

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=C1700103&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

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