

1,4-Cyclooctadiene

Other names:	Cycloocta-1,4-diene
Inchi:	InChI=1S/C8H12/c1-2-4-6-8-7-5-3-1/h1-2,5,7H,3-4,6,8H2/b2-1-,7-5?
InchiKey:	DNZZPKYSGRTNGK-ACALLGSNSA-N
Formula:	C8H12
SMILES:	C1=CCCCC=CC1
Mol. weight [g/mol]:	108.18
CAS:	1073-07-0

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	8.64 ± 0.03	eV	NIST Webbook
ie	8.50	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
tb	413.52	K	Joback Method
tc	637.21	K	Joback Method
tf	220.00 ± 4.00	K	NIST Webbook
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.96	J/molxK	413.52	Joback Method
cpg	200.71	J/molxK	450.80	Joback Method
cpg	216.53	J/molxK	488.08	Joback Method
cpg	231.45	J/molxK	525.37	Joback Method
cpg	245.48	J/molxK	562.65	Joback Method
cpg	258.65	J/molxK	599.93	Joback Method

cpg	270.98	J/mol×K	637.21	Joback Method
dvisc	0.0291355	Paxs	186.02	Joback Method
dvisc	0.0063666	Paxs	223.94	Joback Method
dvisc	0.0021612	Paxs	261.85	Joback Method
dvisc	0.0009642	Paxs	299.77	Joback Method
dvisc	0.0005156	Paxs	337.69	Joback Method
dvisc	0.0003129	Paxs	375.60	Joback Method
dvisc	0.0002081	Paxs	413.52	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38062e+01
Coeff. B	-3.34077e+03
Coeff. C	-5.73960e+01
Temperature range (K), min.	304.52
Temperature range (K), max.	450.67

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=C1073070&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/ci9903071

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

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