1,3,5-Cyclooctatriene

Other names: Cycloocta-1,3,5-triene
Inchi: InChI=1S/C8H10/c1-2-4-6-8-7-5-3-1/h1-6H,7-8H2/b2-1-,5-3-,6-4-
InchiKey: ICPMUWPXCAVOOQ-XCADPSHZSA-N
Formula: C8H10
SMILES: C1=CC=CCCC=C1
Mol. weight [g/mol]: 106.17
CAS: 1871-52-9

Physical Properties

Property code	Value	Unit	Source
gf	114.32	kJ/mol	Joback Method
hf	27.23	kJ/mol	Joback Method
hfus	6.71	kJ/mol	Joback Method
hvap	35.36	kJ/mol	Joback Method
ie	7.90	eV	NIST Webbook
log10ws	-2.63		Crippen Method
logp	2.449		Crippen Method
mcvol	99.820	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
rinpol	905.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	905.00		NIST Webbook
tb	418.70	K	NIST Webbook
tc	638.83	K	Joback Method
tf	189.90 ± 3.00	K	NIST Webbook
tf	183.20 ± 4.00	K	NIST Webbook
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.70	J/mol×K	412.68	Joback Method
cpg	238.69	J/mol×K	601.14	Joback Method
cpg	226.79	J/mol×K	563.45	Joback Method

cpg	214.07	J/mol×K	525.76	Joback Method
cpg	200.49	J/mol×K	488.06	Joback Method
cpg	186.04	J/mol×K	450.37	Joback Method
cpg	249.79	J/mol×K	638.83	Joback Method
dvisc	0.0001978	Pa×s	412.68	Joback Method
dvisc	0.0002902	Pa×s	375.03	Joback Method
dvisc	0.0004637	Pa×s	337.38	Joback Method
dvisc	0.0008336	Pa×s	299.73	Joback Method
dvisc	0.0017735	Pa×s	262.08	Joback Method
dvisc	0.0048607	Pa×s	224.43	Joback Method
dvisc	0.0200035	Pa×s	186.78	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.20	K	12.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42804e+01
Coeff. B	-3.48959e+03
Coeff. C	-5.75350e+01
Temperature range (K), min.	306.92
Temperature range (K), max.	446.61

Sources

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=C1871529&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume