

1,3,6-Cyclooctatriene

Other names:	1,4,6-Cyclooctatriene
Inchi:	InChI=1S/C8H10/c1-2-4-6-8-7-5-3-1/h1-4,7-8H,5-6H2/b3-1-,4-2-,8-7-
InchiKey:	LHNSMWDERKGLJK-DKPWQKSPSA-N
Formula:	C8H10
SMILES:	C1=CCC=CCC=C1
Mol. weight [g/mol]:	106.17
CAS:	3725-30-2

Physical Properties

Property code	Value	Unit	Source
gf	114.32	kJ/mol	Joback Method
hf	196.30	kJ/mol	NIST Webbook
hfus	6.71	kJ/mol	Joback Method
hvap	35.36	kJ/mol	Joback Method
ie	8.50	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
tb	412.68	K	Joback Method
tc	638.83	K	Joback Method
tf	214.00 ± 8.00	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	186.04	J/mol×K	450.37	Joback Method
cpg	200.49	J/mol×K	488.06	Joback Method
cpg	214.07	J/mol×K	525.76	Joback Method
cpg	226.79	J/mol×K	563.45	Joback Method
cpg	238.69	J/mol×K	601.14	Joback Method
cpg	249.79	J/mol×K	638.83	Joback Method

dvisc	0.0200035	Pa×s	186.78	Joback Method
dvisc	0.0048607	Pa×s	224.43	Joback Method
dvisc	0.0017735	Pa×s	262.08	Joback Method
dvisc	0.0008336	Pa×s	299.73	Joback Method
dvisc	0.0004637	Pa×s	337.38	Joback Method
dvisc	0.0002902	Pa×s	375.03	Joback Method
dvisc	0.0001978	Pa×s	412.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.20	K	8.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41591e+01
Coeff. B	-3.43935e+03
Coeff. C	-5.67670e+01
Temperature range (K), min.	304.71
Temperature range (K), max.	445.50

Sources

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=C3725302&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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