1,3,5,7-Cyclooctatetraene

Other names:	Cyclooctatetraene
	UN 2358
	[8]Annulene
Inchi:	InChI=1S/C8H8/c1-2-4-6-8-7-5-3-1/h1-8H/b2-1-,3-1-,4-2-,5-3-,6-4-,7-5-,8-6-,8-7-
InchiKey:	KDUIUFJBNGTBMD-BONZMOEMSA-N
Formula:	C8H8
SMILES:	C1=CC=CC=CC=C1
Mol. weight [g/mol]:	104.15
CAS:	629-20-9

Physical Properties

Property code	Value	Unit	Source
chl	-4539.00 ± 3.00	kJ/mol	NIST Webbook
chl	-4545.92 ± 0.92	kJ/mol	NIST Webbook
ea	0.57 ± 0.03	eV	NIST Webbook
ea	0.55 ± 0.02	eV	NIST Webbook
ea	0.58 ± 0.04	eV	NIST Webbook
ea	0.82	eV	NIST Webbook
ea	0.65 ± 0.04	eV	NIST Webbook
ea	0.58 ± 0.10	eV	NIST Webbook
gf	144.28	kJ/mol	Joback Method
hf	297.60 ± 1.30	kJ/mol	NIST Webbook
hfl	254.50 ± 1.30	kJ/mol	NIST Webbook
hfus	7.93	kJ/mol	Joback Method
hvap	43.10 ± 0.31	kJ/mol	NIST Webbook
hvap	43.10	kJ/mol	NIST Webbook
ie	8.21	eV	NIST Webbook
ie	8.04	eV	NIST Webbook
ie	7.99 ± 0.02	eV	NIST Webbook
ie	8.43	eV	NIST Webbook
ie	8.03	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.225		Crippen Method
mcvol	95.520	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
rinpol	880.00		NIST Webbook

rinpol	850.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	880.00		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1264.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1226.00		NIST Webbook
sg	326.80 ± 1.50	J/mol×K	NIST Webbook
sl	220.29	J/mol×K	NIST Webbook
tb	416.00 ± 4.00	K	NIST Webbook
tb	415.70	K	NIST Webbook
tc	640.50	K	Joback Method
tf	265.00 ± 1.50	K	NIST Webbook
tf	266.00 ± 3.00	K	NIST Webbook
tt	268.48 ± 0.01	K	NIST Webbook
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.49	J/mol×K	640.50	Joback Method
cpg	218.65	J/mol×K	602.39	Joback Method
cpg	157.51	J/mol×K	411.84	Joback Method
cpg	171.42	J/mol×K	449.95	Joback Method
cpg	184.46	J/mol×K	488.06	Joback Method
cpg	196.66	J/mol×K	526.17	Joback Method
cpg	208.05	J/mol×K	564.28	Joback Method
cpl	185.18	J/mol×K	298.15	NIST Webbook
dvisc	0.0002688	Pa×s	374.46	Joback Method
dvisc	0.0001878	Pa×s	411.84	Joback Method
dvisc	0.0137901	Pa×s	187.54	Joback Method
dvisc	0.0037168	Pa×s	224.92	Joback Method

dvisc	0.0014557	Pa×s	262.31	Joback Method
dvisc	0.0007203	Pa×s	299.69	Joback Method
dvisc	0.0004167	Pa×s	337.07	Joback Method
hfust	11.27	kJ/mol	268.50	NIST Webbook
hfust	11.25	kJ/mol	268.50	NIST Webbook
hfust	11.27	kJ/mol	268.48	NIST Webbook
hvapt	43.90	kJ/mol	310.50	NIST Webbook
sfust	41.49	J/mol×K	268.48	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49287e+01
Coeff. B	-3.53287e+03
Coeff. C	-6.08070e+01
Temperature range (K), min.	302.10
Temperature range (K), max.	428.15

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C629209&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

dvisc: Dynamic viscosity

ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
sg:	Molar entropy at standard conditions
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