Bicyclo[4.2.0]octa-1,3,5-triene

Other names:	Benzocyclobutene Benzocyclobutane Benzocyclobutene, 1,2-dihydro- Cardene 1,2-Dihydrobenzocyclobutene
Inchi:	InChI=1S/C8H8/c1-2-4-8-6-5-7(8)3-1/h1-4H,5-6H2
InchiKey:	UMIVXZPTRXBADB-UHFFFAOYSA-N
Formula:	C8H8
SMILES:	c1ccc2c(c1)CC2
Mol. weight [g/mol]:	104.15
CAS:	694-87-1

Physical Properties

Property code	Value	Unit	Source
chl	-4447.00 ± 0.90	kJ/mol	NIST Webbook
gf	199.82	kJ/mol	Joback Method
hf	199.40 ± 0.90	kJ/mol	NIST Webbook
hfl	155.70 ± 0.90	kJ/mol	NIST Webbook
hfus	9.29	kJ/mol	Joback Method
hvap	43.70 ± 0.10	kJ/mol	NIST Webbook
hvap	43.70	kJ/mol	NIST Webbook
ie	8.74 ± 0.05	eV	NIST Webbook
ie	8.66	eV	NIST Webbook
ie	8.66 ± 0.03	eV	NIST Webbook
log10ws	-2.13		Crippen Method
logp	1.785		Crippen Method
mcvol	88.960	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
ripol	1269.00		NIST Webbook
ripol	1272.00		NIST Webbook
ripol	1258.00		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1269.00		NIST Webbook
tb	421.24	K	Joback Method
tc	642.21	K	Joback Method
tf	244.56	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.48	J/mol×K	421.24	Joback Method
cpg	214.81	J/mol×K	605.38	Joback Method
cpg	205.83	J/mol×K	568.55	Joback Method
cpg	196.08	J/mol×K	531.72	Joback Method
cpg	185.49	J/mol×K	494.90	Joback Method
cpg	173.98	J/mol×K	458.07	Joback Method
cpg	223.08	J/mol×K	642.21	Joback Method
dvisc	0.0004112	Pa×s	421.24	Joback Method
dvisc	0.0004548	Pa×s	391.79	Joback Method
dvisc	0.0005113	Pa×s	362.35	Joback Method
dvisc	0.0005868	Pa×s	332.90	Joback Method
dvisc	0.0006917	Pa×s	303.45	Joback Method
dvisc	0.0008447	Pa×s	274.01	Joback Method
dvisc	0.0010825	Pa×s	244.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	323.80 ± 0.20	K	2.70	NIST Webbook

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=C694871&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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
ripol:	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

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