

Bicyclo[4.1.0]hepta-1,3,5-triene

Other names:	1,3,5-Norcaratriene Benzocyclopropene Cyclopropabenzene
Inchi:	InChI=1S/C7H6/c1-2-4-7-5-6(7)3-1/h1-4H,5H2
InchiKey:	AMSMVCOBCOZLEE-UHFFFAOYSA-N
Formula:	C7H6
SMILES:	c1ccc2c(c1)C2
Mol. weight [g/mol]:	90.12
CAS:	4646-69-9

Physical Properties

Property code	Value	Unit	Source
gf	203.50	kJ/mol	Joback Method
hf	142.71	kJ/mol	Joback Method
hfus	8.80	kJ/mol	Joback Method
hvap	33.99	kJ/mol	Joback Method
ie	8.82	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
log10ws	-1.82		Crippen Method
logp	1.591		Crippen Method
mcvol	74.870	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	394.09	K	Joback Method
tc	608.35	K	Joback Method
tf	236.81	K	Joback Method
vc	0.293	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.30	J/molxK	394.09	Joback Method
cpg	136.71	J/molxK	429.80	Joback Method
cpg	146.21	J/molxK	465.51	Joback Method
cpg	154.87	J/molxK	501.22	Joback Method

cpg	162.78	J/mol×K	536.93	Joback Method
cpg	169.99	J/mol×K	572.64	Joback Method
cpg	176.59	J/mol×K	608.35	Joback Method
dvisc	0.0006123	Paxs	236.81	Joback Method
dvisc	0.0005496	Paxs	263.02	Joback Method
dvisc	0.0005030	Paxs	289.24	Joback Method
dvisc	0.0004673	Paxs	315.45	Joback Method
dvisc	0.0004390	Paxs	341.66	Joback Method
dvisc	0.0004161	Paxs	367.88	Joback Method
dvisc	0.0003972	Paxs	394.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C4646699&Units=SI

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

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