CYCLOPROPABENZENE

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

Physical Properties

Property code	Value	Unit	Source
af	0.3371		Cheméo Relay (1.0)
gf	203.50	kJ/mol	Joback Method
hf	155.83	kJ/mol	Cheméo Relay (1.0)
hfus	8.80	kJ/mol	Joback Method
hvap	35.04	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
log10ws	-2.85		Cheméo Relay (1.0)
logp	1.591		Crippen Method
mcvol	74.870	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	428.54	K	Cheméo Relay (1.0)
tc	644.07	K	Cheméo Relay (1.0)
tf	266.70	K	Cheméo Relay (1.0)
vc	0.289	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.30	J/mol×K	394.09	Joback Method
cpg	136.71	J/mol×K	429.80	Joback Method
cpg	146.21	J/mol×K	465.51	Joback Method
cpg	154.87	J/mol×K	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	Pa×s	236.81	Joback Method
dvisc	0.0005496	Pa×s	263.02	Joback Method
dvisc	0.0005030	Pa×s	289.24	Joback Method
dvisc	0.0004673	Pa×s	315.45	Joback Method
dvisc	0.0004390	Pa×s	341.66	Joback Method
dvisc	0.0004161	Pa×s	367.88	Joback Method
dvisc	0.0003972	Pa×s	394.09	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4646699&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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