1,4-Ethenonaphthalene, 1,4-dihydro-

Other names:	Benzobarrelene
	Benzobicyclo[2.2.2]octatriene
Inchi:	InChI=1S/C12H10/c1-2-4-12-10-7-5-9(6-8-10)11(12)3-1/h1-10H
InchiKey:	HQFAAEWHTFVMMR-UHFFFAOYSA-N
Formula:	C12H10
SMILES:	C1=CC2C=CC1c1ccccc12
Mol. weight [g/mol]:	154.21
CAS:	7322-47-6

Physical Properties

Property code	Value	Unit	Source
gf	334.36	kJ/mol	Joback Method
hf	195.21	kJ/mol	Joback Method
hfus	19.20	kJ/mol	Joback Method
hvap	45.65	kJ/mol	Joback Method
ie	8.12	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-3.34		Crippen Method
logp	2.993		Crippen Method
mcvol	125.860	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	517.42	K	Joback Method
tc	756.04	K	Joback Method
tf	301.34	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.96	J/mol×K	517.42	Joback Method
cpg	299.10	J/mol×K	557.19	Joback Method
cpg	313.84	J/mol×K	596.96	Joback Method
cpg	327.32	J/mol×K	636.73	Joback Method
cpg	339.65	J/mol×K	676.50	Joback Method

cpg	350.98	J/mol×K	716.27	Joback Method
cpg	361.42	J/mol×K	756.04	Joback Method
dvisc	0.0011225	Pa×s	301.34	Joback Method
dvisc	0.0010459	Pa×s	337.35	Joback Method
dvisc	0.0009880	Pa×s	373.37	Joback Method
dvisc	0.0009427	Pa×s	409.38	Joback Method
dvisc	0.0009063	Pa×s	445.39	Joback Method
dvisc	0.0008764	Pa×s	481.41	Joback Method
dvisc	0.0008515	Pa×s	517.42	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7322476&Units=SI
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

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