5,6,7,8,9,10-Hexahydrobenzocyclooctene

Other names: Benzocyclooctene,5,6,7,8,9,10-hexahydro-
Inchi: InChI=1S/C12H16/c1-2-4-8-12-10-6-5-9-11(12)7-3-1/h5-6,9-10H,1-4,7-8H2
InchiKey: ADKYNRATSQVVPJ-UHFFFAOYSA-N
Formula: C12H16
SMILES: c1ccc2c(c1)CCCCCC2
Mol. weight [g/mol]: 160.26
CAS: 1076-69-3

Physical Properties

Property code	Value	Unit	Source
gf	185.10	kJ/mol	Joback Method
hf	8.71	kJ/mol	Joback Method
hfus	11.25	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
ie	8.97 ± 0.03	eV	NIST Webbook
ie	8.42	eV	NIST Webbook
log10ws	-3.81		Crippen Method
logp	3.346		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	529.84	K	Joback Method
tc	771.90	K	Joback Method
tf	275.56	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.74	J/mol×K	529.84	Joback Method
cpg	353.15	J/mol×K	570.18	Joback Method
cpg	372.13	J/mol×K	610.53	Joback Method
cpg	389.74	J/mol×K	650.87	Joback Method
cpg	406.06	J/mol×K	691.21	Joback Method
cpg	421.16	J/mol×K	731.55	Joback Method

cpg	435.09	J/mol×K	771.90	Joback Method
dvisc	0.0045845	Pa×s	275.56	Joback Method
dvisc	0.0019244	Pa×s	317.94	Joback Method
dvisc	0.0009908	Pa×s	360.32	Joback Method
dvisc	0.0005867	Pa×s	402.70	Joback Method
dvisc	0.0003838	Pa×s	445.08	Joback Method
dvisc	0.0002703	Pa×s	487.46	Joback Method
dvisc	0.0002014	Pa×s	529.84	Joback Method

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=C1076693&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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