5H-Benzocycloheptene,6,7,8,9-tetrahydro-

Other names: Benzocycloheptene
Inchi: InChI=1S/C11H14/c1-2-6-10-8-4-5-9-11(10)7-3-1/h4-5,8-9H,1-3,6-7H2
InchiKey: HEOQXHNKRXRCTO-UHFFFAOYSA-N
Formula: C11H14
SMILES: c1ccc2c(c1)CCCCC2
Mol. weight [g/mol]: 146.23
CAS: 1075-16-7

Physical Properties

Property code	Value	Unit	Source
gf	188.78	kJ/mol	Joback Method
hf	35.51	kJ/mol	Joback Method
hfus	10.76	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
ie	8.40 ± 0.02	eV	NIST Webbook
ie	8.44	eV	NIST Webbook
ie	9.10 ± 0.05	eV	NIST Webbook
log10ws	-3.39		Crippen Method
logp	2.956		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	502.69	K	Joback Method
tc	740.24	K	Joback Method
tf	267.81	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.58	J/mol×K	502.69	Joback Method
cpg	366.02	J/mol×K	700.65	Joback Method
cpg	352.26	J/mol×K	661.06	Joback Method
cpg	337.40	J/mol×K	621.46	Joback Method
cpg	321.38	J/mol×K	581.87	Joback Method

cpg	304.13	J/mol×K	542.28	Joback Method
cpg	378.75	J/mol×K	740.24	Joback Method
dvisc	0.0002658	Pa×s	502.69	Joback Method
dvisc	0.0003412	Pa×s	463.54	Joback Method
dvisc	0.0004587	Pa×s	424.40	Joback Method
dvisc	0.0006549	Pa×s	385.25	Joback Method
dvisc	0.0010133	Pa×s	346.10	Joback Method
dvisc	0.0017526	Pa×s	306.96	Joback Method
dvisc	0.0035581	Pa×s	267.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1075167&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