Benzobicyclo[2.2.0]hexa-2,5-diene

Inchi: InChI=1S/C10H8/c1-2-4-8-7(3-1)9-5-6-10(8)9/h1-6,9-10H
InchiKey: JYKMWOMRHHJZMI-UHFFFAOYSA-N
Formula: C10H8
SMILES: C1=CC2c3ccccc3C12
Mol. weight [g/mol]: 128.17
CAS: 20847-82-9

Physical Properties

Property code	Value	Unit	Source
gf	311.76	kJ/mol	Joback Method
hf	399.00 ± 7.90	kJ/mol	NIST Webbook
hfus	17.00	kJ/mol	Joback Method
hvap	40.57	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.437		Crippen Method
mcvol	101.980	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	463.96	K	Joback Method
tc	690.23	K	Joback Method
tf	285.08	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.74	J/mol×K	463.96	Joback Method
cpg	271.95	J/mol×K	652.52	Joback Method
cpg	262.37	J/mol×K	614.81	Joback Method
cpg	251.88	J/mol×K	577.10	Joback Method
cpg	240.36	J/mol×K	539.38	Joback Method
cpg	227.69	J/mol×K	501.67	Joback Method
cpg	280.73	J/mol×K	690.23	Joback Method
dvisc	0.0009836	Pa×s	463.96	Joback Method
dvisc	0.0009381	Pa×s	434.15	Joback Method

dvisc	0.0008885	Pa×s	404.33	Joback Method
dvisc	0.0008342	Pa×s	374.52	Joback Method
dvisc	0.0007748	Pa×s	344.71	Joback Method
dvisc	0.0007096	Pa×s	314.89	Joback Method
dvisc	0.0006381	Pa×s	285.08	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20847829&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
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