Bicyclo[3.2.0]hepta-2,6-diene

Inchi: InChI=1S/C7H8/c1-2-6-4-5-7(6)3-1/h1-2,4-7H,3H2
InchiKey: PZWQRDVVVKIYLX-UHFFFAOYSA-N
Formula: C7H8
SMILES: C1=CC2C=CC2C1
Mol. weight [g/mol]: 92.14
CAS: 2422-86-8

Physical Properties

Property code	Value	Unit	Source
gf	177.38	kJ/mol	Joback Method
hf	264.00	kJ/mol	NIST Webbook
hfus	10.50	kJ/mol	Joback Method
hvap	31.76	kJ/mol	Joback Method
ie	8.92	eV	NIST Webbook
ie	8.35	eV	NIST Webbook
ie	8.35	eV	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.748		Crippen Method
mcvol	79.170	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
tb	375.63	K	Joback Method
tc	582.98	K	Joback Method
tf	202.53	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.22	J/mol×K	375.63	Joback Method
cpg	194.97	J/mol×K	548.42	Joback Method
cpg	184.97	J/mol×K	513.86	Joback Method
cpg	174.16	J/mol×K	479.30	Joback Method
cpg	162.48	J/mol×K	444.75	Joback Method
cpg	149.85	J/mol×K	410.19	Joback Method

cpg	204.21	J/mol×K	582.98	Joback Method
dvisc	0.0003745	Pa×s	375.63	Joback Method
dvisc	0.0003712	Pa×s	346.78	Joback Method
dvisc	0.0003673	Pa×s	317.93	Joback Method
dvisc	0.0003627	Pa×s	289.08	Joback Method
dvisc	0.0003571	Pa×s	260.23	Joback Method
dvisc	0.0003503	Pa×s	231.38	Joback Method
dvisc	0.0003417	Pa×s	202.53	Joback Method

Sources

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=C2422868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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