Bicyclo[3.2.1]octa-2,6-diene

Inchi: InChI=1S/C8H10/c1-2-7-4-5-8(3-1)6-7/h1-2,4-5,7-8H,3,6H2
InchiKey: VTYQQMGYHHVPMX-UHFFFAOYSA-N
Formula: C8H10
SMILES: C1=CC2C=CC(C1)C2
Mol. weight [g/mol]: 106.17
CAS: 4096-95-1

Physical Properties

Property code	Value	Unit	Source
gf	173.70	kJ/mol	Joback Method
hf	159.00 ± 6.30	kJ/mol	NIST Webbook
hf	158.00 ± 0.80	kJ/mol	NIST Webbook
hfl	120.00 ± 3.00	kJ/mol	NIST Webbook
hfus	10.99	kJ/mol	Joback Method
hvap	39.00	kJ/mol	NIST Webbook
ie	8.44 ± 0.01	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	2.139		Crippen Method
mcvol	93.260	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	402.78	K	Joback Method
tc	617.25	K	Joback Method
tf	210.28	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.91	J/mol×K	402.78	Joback Method
cpg	188.64	J/mol×K	438.53	Joback Method
cpg	203.27	J/mol×K	474.27	Joback Method
cpg	216.87	J/mol×K	510.02	Joback Method
cpg	229.50	J/mol×K	545.76	Joback Method
cpg	241.22	J/mol×K	581.51	Joback Method

cpg	252.10	J/mol×K	617.25	Joback Method
dvisc	0.0007709	Pa×s	210.28	Joback Method
dvisc	0.0006515	Pa×s	242.36	Joback Method
dvisc	0.0005727	Pa×s	274.45	Joback Method
dvisc	0.0005172	Pa×s	306.53	Joback Method
dvisc	0.0004762	Pa×s	338.61	Joback Method
dvisc	0.0004447	Pa×s	370.70	Joback Method
dvisc	0.0004199	Pa×s	402.78	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4096951&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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