Bicyclo(3.3.1)non-2-ene

Inchi: InChI=1S/C9H14/c1-3-8-5-2-6-9(4-1)7-8/h1,3,8-9H,2,4-7H2
InchiKey: CEVDPSDZXGCLEI-UHFFFAOYSA-N
Formula: C9H14
SMILES: C1=CC2CCCC(C1)C2
Mol. weight [g/mol]: 122.21
CAS: 6671-66-5

Physical Properties

Property code	Value	Unit	Source
chs	-5445.10 ± 1.30	kJ/mol	NIST Webbook
gf	140.06	kJ/mol	Joback Method
hf	-49.10 ± 1.40	kJ/mol	NIST Webbook
hfs	-97.30 ± 1.30	kJ/mol	NIST Webbook
hfus	10.26	kJ/mol	Joback Method
hsub	48.20 ± 0.40	kJ/mol	NIST Webbook
hsub	48.20	kJ/mol	NIST Webbook
hsub	48.20 ± 0.40	kJ/mol	NIST Webbook
hvap	36.26	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.753		Crippen Method
mcvol	111.650	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
tb	430.77	K	Joback Method
tc	649.36	K	Joback Method
tf	217.27	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.80	J/mol×K	430.77	Joback Method
cpg	310.78	J/mol×K	612.93	Joback Method
cpg	296.19	J/mol×K	576.50	Joback Method
cpg	280.56	J/mol×K	540.06	Joback Method

cpg	263.83	J/mol×K	503.63	Joback Method
cpg	245.93	J/mol×K	467.20	Joback Method
cpg	324.39	J/mol×K	649.36	Joback Method
dvisc	0.0004387	Pa×s	430.77	Joback Method
dvisc	0.0005047	Pa×s	395.19	Joback Method
dvisc	0.0005970	Pa×s	359.60	Joback Method
dvisc	0.0007327	Pa×s	324.02	Joback Method
dvisc	0.0009458	Pa×s	288.44	Joback Method
dvisc	0.0013118	Pa×s	252.85	Joback Method
dvisc	0.0020254	Pa×s	217.27	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6671665&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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