Bicyclo[3.3.1]nonane

Inchi: InChI=1S/C9H16/c1-3-8-5-2-6-9(4-1)7-8/h8-9H,1-7H2
InchiKey: WNTGVOIBBXFMLR-UHFFFAOYSA-N
Formula: C9H16
SMILES: C1CC2CCCC(C1)C2
Mol. weight [g/mol]: 124.22
CAS: 280-65-9

Physical Properties

Property code	Value	Unit	Source
chs	-5650.10 ± 0.80	kJ/mol	NIST Webbook
gf	110.10	kJ/mol	Joback Method
hf	-128.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-178.00 ± 0.80	kJ/mol	NIST Webbook
hfus	9.04	kJ/mol	Joback Method
hsub	50.00	kJ/mol	NIST Webbook
hsub	51.00 ± 2.00	kJ/mol	NIST Webbook
hvap	35.97	kJ/mol	Joback Method
ie	9.35	eV	NIST Webbook
log10ws	-2.90		Crippen Method
logp	2.977		Crippen Method
mcvol	115.950	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
tb	431.61	K	Joback Method
tc	647.88	K	Joback Method
tf	216.51	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.88	J/mol×K	647.88	Joback Method
cpg	331.12	J/mol×K	611.84	Joback Method
cpg	315.35	J/mol×K	575.79	Joback Method
cpg	298.50	J/mol×K	539.75	Joback Method

cpg	280.52	J/mol×K	503.70	Joback Method
cpg	261.35	J/mol×K	467.66	Joback Method
cpg	240.94	J/mol×K	431.61	Joback Method
dvisc	0.0026731	Pa×s	216.51	Joback Method
dvisc	0.0004581	Pa×s	431.61	Joback Method
dvisc	0.0005380	Pa×s	395.76	Joback Method
dvisc	0.0006525	Pa×s	359.91	Joback Method
dvisc	0.0008258	Pa×s	324.06	Joback Method
dvisc	0.0011082	Pa×s	288.21	Joback Method
dvisc	0.0016168	Pa×s	252.36	Joback Method
hsubt	51.00 ± 2.00	kJ/mol	290.00	NIST Webbook

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=C280659&Units=SI

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
hsubt: Enthalpy of sublimation at a given temperature
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