

Bicyclo[4,2,1]non-3-ene

Inchi: InChI=1S/C9H14/c1-2-4-9-6-5-8(3-1)7-9/h1-2,8-9H,3-7H2
InchiKey: VQBSXAZGFWSWHD-UHFFFAOYSA-N
Formula: C9H14
SMILES: C1=CCC2CCC(C1)C2
Mol. weight [g/mol]: 122.21
CAS: 16456-33-0

Physical Properties

Property code	Value	Unit	Source
chs	-5496.30 ± 0.90	kJ/mol	NIST Webbook
gf	140.06	kJ/mol	Joback Method
hf	3.60 ± 1.20	kJ/mol	NIST Webbook
hfs	-46.10 ± 0.90	kJ/mol	NIST Webbook
hfus	10.26	kJ/mol	Joback Method
hsub	49.70 ± 0.80	kJ/mol	NIST Webbook
hsub	49.70	kJ/mol	NIST Webbook
hsub	49.70 ± 0.80	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	245.93	J/mol×K	467.20	Joback Method
cpg	263.83	J/mol×K	503.63	Joback Method
cpg	280.56	J/mol×K	540.06	Joback Method

cpg	296.19	J/mol×K	576.50	Joback Method
cpg	310.78	J/mol×K	612.93	Joback Method
cpg	324.39	J/mol×K	649.36	Joback Method
dvisc	0.0020254	Pa×s	217.27	Joback Method
dvisc	0.0013118	Pa×s	252.85	Joback Method
dvisc	0.0009458	Pa×s	288.44	Joback Method
dvisc	0.0007327	Pa×s	324.02	Joback Method
dvisc	0.0005970	Pa×s	359.60	Joback Method
dvisc	0.0005047	Pa×s	395.19	Joback Method
dvisc	0.0004387	Pa×s	430.77	Joback Method

Sources

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=C16456330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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