

Bicyclo[4.2.1]non-1(2)-ene

Inchi:	InChI=1S/C9H14/c1-2-4-9-6-5-8(3-1)7-9/h3,9H,1-2,4-7H2
InchiKey:	BFHUIVOGLJUQID-UHFFFAOYSA-N
Formula:	C9H14
SMILES:	C1=C2CCC(CCC1)C2
Mol. weight [g/mol]:	122.21
CAS:	23057-36-5

Physical Properties

Property code	Value	Unit	Source
gf	138.14	kJ/mol	Joback Method
hf	73.60	kJ/mol	NIST Webbook
hfus	8.80	kJ/mol	Joback Method
hvap	37.23	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.897		Crippen Method
mcvol	111.650	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	440.42	K	Joback Method
tc	660.88	K	Joback Method
tf	234.03	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.36	J/molxK	440.42	Joback Method
cpg	308.17	J/molxK	624.13	Joback Method
cpg	294.33	J/molxK	587.39	Joback Method
cpg	279.48	J/molxK	550.65	Joback Method
cpg	263.58	J/molxK	513.91	Joback Method
cpg	246.56	J/molxK	477.16	Joback Method
cpg	321.09	J/molxK	660.88	Joback Method
dvisc	0.0004287	Paxs	440.42	Joback Method
dvisc	0.0005065	Paxs	406.02	Joback Method

dvisc	0.0006172	Paxs	371.62	Joback Method
dvisc	0.0007830	Paxs	337.22	Joback Method
dvisc	0.0010486	Paxs	302.83	Joback Method
dvisc	0.0015134	Paxs	268.43	Joback Method
dvisc	0.0024329	Paxs	234.03	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=C23057365&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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