

Bicyclo[2.2.2]oct-2-ene,5-methylene-

Inchi:	InChI=1S/C9H12/c1-7-6-8-2-4-9(7)5-3-8/h2,4,8-9H,1,3,5-6H2
InchiKey:	XERADROWVPYPEM-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	C=C1CC2C=CC1CC2
Mol. weight [g/mol]:	120.19
CAS:	19386-05-1

Physical Properties

Property code	Value	Unit	Source
gf	205.24	kJ/mol	Joback Method
hf	46.21	kJ/mol	Joback Method
hfus	11.20	kJ/mol	Joback Method
hvap	36.25	kJ/mol	Joback Method
ie	8.97	eV	NIST Webbook
log10ws	-2.60		Crippen Method
logp	2.529		Crippen Method
mcvol	107.350	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
rinpol	783.00		NIST Webbook
tb	425.66	K	Joback Method
tc	637.47	K	Joback Method
tf	234.47	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.90	J/molxK	425.66	Joback Method
cpg	285.87	J/molxK	602.17	Joback Method
cpg	273.34	J/molxK	566.87	Joback Method
cpg	259.93	J/molxK	531.57	Joback Method
cpg	245.59	J/molxK	496.26	Joback Method
cpg	230.26	J/molxK	460.96	Joback Method
cpg	297.58	J/molxK	637.47	Joback Method

dvisc	0.0004906	Paxs	425.66	Joback Method
dvisc	0.0005198	Paxs	393.79	Joback Method
dvisc	0.0005565	Paxs	361.93	Joback Method
dvisc	0.0006036	Paxs	330.06	Joback Method
dvisc	0.0006662	Paxs	298.20	Joback Method
dvisc	0.0007529	Paxs	266.33	Joback Method
dvisc	0.0008795	Paxs	234.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19386051&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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