

Bicyclo[2.2.2]oct-2-ene

Other names:	Bicyclo[2.2.2]octene Cyclohexene, 3,6-endo-(1,2-ethanediyl)- 3,6-Endoethylenecyclohexene 2,2,2-Bicyclooctene-2 Bicyclo[2.2.2]-2-octene Bicyclo[2,2,2]-2-octene
Inchi:	InChI=1S/C8H12/c1-2-8-5-3-7(1)4-6-8/h1-2,7-8H,3-6H2
InchiKey:	VIQRCOQXIHJND-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	C1=CC2CCC1CC2
Mol. weight [g/mol]:	108.18
CAS:	931-64-6

Physical Properties

Property code	Value	Unit	Source
chs	-4839.72 ± 0.67	kJ/mol	NIST Webbook
gf	143.74	kJ/mol	Joback Method
hf	26.00	kJ/mol	NIST Webbook
hf	20.40 ± 0.79	kJ/mol	NIST Webbook
hfs	-23.00 ± 0.67	kJ/mol	NIST Webbook
hfus	9.77	kJ/mol	Joback Method
hsub	43.40	kJ/mol	NIST Webbook
hvap	33.86	kJ/mol	Joback Method
ie	9.07	eV	NIST Webbook
ie	9.05 ± 0.02	eV	NIST Webbook
ie	8.92	eV	NIST Webbook
ie	9.03	eV	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.363		Crippen Method
mcvol	97.560	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
sg	316.30	J/mol×K	NIST Webbook
ss	210.46	J/mol×K	NIST Webbook
tb	404.00 ± 3.00	K	NIST Webbook
tc	615.80	K	Joback Method
tf	384.50 ± 0.50	K	NIST Webbook
tt	389.75 ± 0.01	K	NIST Webbook

vc	0.367	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.77	J/mol×K	403.62	Joback Method
cpg	202.83	J/mol×K	438.98	Joback Method
cpg	218.77	J/mol×K	474.35	Joback Method
cpg	233.66	J/mol×K	509.71	Joback Method
cpg	247.55	J/mol×K	545.07	Joback Method
cpg	260.50	J/mol×K	580.43	Joback Method
cpg	272.57	J/mol×K	615.80	Joback Method
cps	156.73	J/mol×K	298.15	NIST Webbook
dvisc	0.0010286	Pa×s	209.52	Joback Method
dvisc	0.0008159	Pa×s	241.87	Joback Method
dvisc	0.0006835	Pa×s	274.22	Joback Method
dvisc	0.0005944	Pa×s	306.57	Joback Method
dvisc	0.0005308	Pa×s	338.92	Joback Method
dvisc	0.0004835	Pa×s	371.27	Joback Method
dvisc	0.0004471	Pa×s	403.62	Joback Method
hfust	5.40	kJ/mol	389.80	NIST Webbook

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=C931646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
sg:	Molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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