

Bicyclo[2.2.1]hept-2-ene, 2-methyl-

Other names:	2-Norbornene, 2-methyl- 2-Methyl-2-norbornene 2-Methylbicyclo[2.2.1]hept-2-ene 2-Methylnorbornene 2-Methylbicyclo(2.2.1)heptene
Inchi:	InChI=1S/C8H12/c1-6-4-7-2-3-8(6)5-7/h4,7-8H,2-3,5H2,1H3
InchiKey:	HTENSGOZPYEMCG-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	CC1=CC2CCC1C2
Mol. weight [g/mol]:	108.18
CAS:	694-92-8

Physical Properties

Property code	Value	Unit	Source
affp	845.00	kJ/mol	NIST Webbook
basg	812.50	kJ/mol	NIST Webbook
chl	-4867.50 ± 1.70	kJ/mol	NIST Webbook
gf	146.21	kJ/mol	Joback Method
hf	-22.70	kJ/mol	Joback Method
hfl	4.40 ± 1.80	kJ/mol	NIST Webbook
hfus	11.48	kJ/mol	Joback Method
hvap	34.35	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.363		Crippen Method
mcvol	97.560	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	1097.00		NIST Webbook
rinpol	1097.00		NIST Webbook
tb	391.00 ± 2.00	K	NIST Webbook
tc	609.36	K	Joback Method
tf	225.56	K	Joback Method
vc	0.376	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.08	J/molxK	404.33	Joback Method
cpg	204.54	J/molxK	438.50	Joback Method
cpg	219.03	J/molxK	472.67	Joback Method
cpg	232.58	J/molxK	506.84	Joback Method
cpg	245.27	J/molxK	541.02	Joback Method
cpg	257.14	J/molxK	575.19	Joback Method
cpg	268.25	J/molxK	609.36	Joback Method
dvisc	0.0005626	Paxs	225.56	Joback Method
dvisc	0.0005347	Paxs	255.35	Joback Method
dvisc	0.0005136	Paxs	285.15	Joback Method
dvisc	0.0004971	Paxs	314.94	Joback Method
dvisc	0.0004838	Paxs	344.74	Joback Method
dvisc	0.0004730	Paxs	374.53	Joback Method
dvisc	0.0004639	Paxs	404.33	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=C694928&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid 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
hfl:	Liquid phase 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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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