2-Methylenebicyclo[2.2.1]-heptane

Other names: Bicyclo[2.2.1]heptane,2-methylene-
Norbornane, 2-methylene-
2-Methylenenorbornane
Inchi: InChI=1S/C8H12/c1-6-4-7-2-3-8(6)5-7/h7-8H,1-5H2
InchiKey: AJQVASAUQUTVJK-UHFFFAOYSA-N
Formula: C8H12
SMILES: C=C1CC2CCC1C2
Mol. weight [g/mol]: 108.18
CAS: 497-35-8

Physical Properties

Property code	Value	Unit	Source
affp	860.70	kJ/mol	NIST Webbook
basg	831.80	kJ/mol	NIST Webbook
chl	-4859.00 ± 1.60	kJ/mol	NIST Webbook
gf	178.96	kJ/mol	Joback Method
hf	15.23	kJ/mol	Joback Method
hfl	-4.10 ± 1.70	kJ/mol	NIST Webbook
hfus	9.49	kJ/mol	Joback Method
hvap	33.56	kJ/mol	Joback Method
ie	9.04	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.363		Crippen Method
mcvol	97.560	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	399.35	K	Joback Method
tc	602.57	K	Joback Method
tf	225.96	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	187.62	J/mol×K	399.35	Joback Method
cpg	256.55	J/mol×K	568.70	Joback Method
cpg	244.50	J/mol×K	534.83	Joback Method
cpg	231.63	J/mol×K	500.96	Joback Method
cpg	217.89	J/mol×K	467.09	Joback Method
cpg	203.24	J/mol×K	433.22	Joback Method
cpg	267.85	J/mol×K	602.57	Joback Method
dvisc	0.0004993	Pa×s	399.35	Joback Method
dvisc	0.0005084	Pa×s	370.45	Joback Method
dvisc	0.0005194	Pa×s	341.55	Joback Method
dvisc	0.0005326	Pa×s	312.66	Joback Method
dvisc	0.0005490	Pa×s	283.76	Joback Method
dvisc	0.0005698	Pa×s	254.86	Joback Method
dvisc	0.0005970	Pa×s	225.96	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C497358&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume