Bicyclo[2.1.1]hex-2-ene

Inchi: InChI=1S/C6H8/c1-2-6-3-5(1)4-6/h1-2,5-6H,3-4H2
InchiKey: YWDBHFZUBPOPRQ-UHFFFAOYSA-N
Formula: C6H8
SMILES: C1=CC2CC1C2
Mol. weight [g/mol]: 80.13
CAS: 822-41-3

Physical Properties

Property code	Value	Unit	Source
gf	151.10	kJ/mol	Joback Method
hf	251.00	kJ/mol	NIST Webbook
hfus	8.79	kJ/mol	Joback Method
hvap	29.07	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.582		Crippen Method
mcvol	69.380	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	349.32	K	Joback Method
tc	546.69	K	Joback Method
tf	194.02	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	113.13	J/mol×K	349.32	Joback Method
cpg	168.72	J/mol×K	513.79	Joback Method
cpg	159.24	J/mol×K	480.90	Joback Method
cpg	148.99	J/mol×K	448.00	Joback Method
cpg	137.93	J/mol×K	415.11	Joback Method
cpg	125.99	J/mol×K	382.21	Joback Method
cpg	177.51	J/mol×K	546.69	Joback Method
dvisc	0.0003230	Pa×s	349.32	Joback Method
dvisc	0.0003049	Pa×s	323.44	Joback Method

dvisc	0.0002849	Pa×s	297.55	Joback Method
dvisc	0.0002628	Pa×s	271.67	Joback Method
dvisc	0.0002383	Pa×s	245.79	Joback Method
dvisc	0.0002112	Pa×s	219.90	Joback Method
dvisc	0.0001813	Pa×s	194.02	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=C822413&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume