

Spirohex-1-ene

Inchi:	InChI=1S/C6H8/c1-2-6(3-1)4-5-6/h4-5H,1-3H2
InchiKey:	MTADUJBFHBFCHU-UHFFFAOYSA-N
Formula:	C6H8
SMILES:	C1=CC12CCC2
Mol. weight [g/mol]:	80.13
CAS:	71153-32-7

Physical Properties

Property code	Value	Unit	Source
gf	153.32	kJ/mol	Joback Method
hf	71.79	kJ/mol	Joback Method
hfus	1.42	kJ/mol	Joback Method
hvap	28.23	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	-1.74		Crippen Method
logp	1.727		Crippen Method
mcvol	69.380	ml/mol	McGowan Method
pc	4959.33	kPa	Joback Method
tb	354.23	K	Joback Method
tc	562.03	K	Joback Method
tf	222.16	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.69	J/molxK	354.23	Joback Method
cpg	126.63	J/molxK	388.86	Joback Method
cpg	139.06	J/molxK	423.50	Joback Method
cpg	150.12	J/molxK	458.13	Joback Method
cpg	159.96	J/molxK	492.76	Joback Method
cpg	168.73	J/molxK	527.40	Joback Method
cpg	176.58	J/molxK	562.03	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=C71153327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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