Spirohexane

Inchi: InChI=1S/C6H10/c1-2-6(3-1)4-5-6/h1-5H2
InchiKey: FYGUBWKMMCWIKB-UHFFFAOYSA-N
Formula: C6H10
SMILES: C1CC2(C1)CC2
Mol. weight [g/mol]: 82.14
CAS: 157-45-9

Physical Properties

Property code	Value	Unit	Source
gf	123.36	kJ/mol	Joback Method
hf	14.01	kJ/mol	Joback Method
hfus	0.20	kJ/mol	Joback Method
hvap	27.93	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
ie	9.66	eV	NIST Webbook
log10ws	-1.88		Crippen Method
logp	1.950		Crippen Method
mcvol	73.680	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	355.07	K	Joback Method
tc	560.61	K	Joback Method
tf	221.40	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.36	J/mol×K	355.07	Joback Method
cpg	138.65	J/mol×K	389.33	Joback Method
cpg	152.43	J/mol×K	423.58	Joback Method
cpg	164.82	J/mol×K	457.84	Joback Method
cpg	175.98	J/mol×K	492.10	Joback Method
cpg	186.04	J/mol×K	526.35	Joback Method
cpg	195.15	J/mol×K	560.61	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=C157459&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
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