Spiro[4.4]non-1-ene

Other names:	Spiro[4.4]nonene
Inchi:	InChI=1S/C9H14/c1-2-6-9(5-1)7-3-4-8-9/h1,5H,2-4,6-8H2
InchiKey:	RWXPSIRAVCNFPR-UHFFFAOYSA-N
Formula:	C9H14
SMILES:	C1=CC2(CC1)CCCC2
Mol. weight [g/mol]:	122.21
CAS:	873-12-1

Physical Properties

Property code	Value	Unit	Source
gf	142.28	kJ/mol	Joback Method
hf	-8.61	kJ/mol	Joback Method
hfus	2.89	kJ/mol	Joback Method
hvap	35.42	kJ/mol	Joback Method
ie	8.73	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
log10ws	-2.99		Crippen Method
logp	2.897		Crippen Method
mcvol	111.650	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	435.68	K	Joback Method
tc	664.87	K	Joback Method
tf	245.41	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.61	J/mol×K	435.68	Joback Method
cpg	246.92	J/mol×K	473.88	Joback Method
cpg	264.54	J/mol×K	512.08	Joback Method
cpg	280.64	J/mol×K	550.28	Joback Method
cpg	295.40	J/mol×K	588.48	Joback Method
cpg	309.00	J/mol×K	626.67	Joback Method

cpg	321.61	J/mol×K	664.87	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=C873121&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

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