Tetracyclo[4.2.2.2^{2,5}.0^{1,6}

Other names: Tetracyclo[4.2.2.2
Inchi: InChI=1S/C12H14/c1-2-10-4-3-9(1)11-5-7-12(10,11)8-6-11/h5-10H,1-4H2
InchiKey: XGOOVFGSWURYBE-UHFFFAOYSA-N
Formula: C12H14
SMILES: C1=CC23C=CC12C1CCC3CC1
Mol. weight [g/mol]: 158.24
CAS: 106697-43-2

Physical Properties

Property code	Value	Unit	Source
gf	342.10	kJ/mol	Joback Method
hf	146.23	kJ/mol	Joback Method
hfus	9.22	kJ/mol	Joback Method
hvap	40.24	kJ/mol	Joback Method
ie	8.85	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-3.17		Crippen Method
logp	2.919		Crippen Method
mcvol	127.900	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	499.72	K	Joback Method
tc	740.60	K	Joback Method
tf	346.08	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.30	J/mol×K	499.72	Joback Method
cpg	339.88	J/mol×K	539.87	Joback Method
cpg	357.16	J/mol×K	580.01	Joback Method
cpg	372.57	J/mol×K	620.16	Joback Method
cpg	386.57	J/mol×K	660.30	Joback Method
cpg	399.58	J/mol×K	700.45	Joback Method

cpg	412.04	J/mol×K	740.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106697432&Units=SI
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

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