12,12-Dimethyl-11-methylenebicyclo[4.4.1]undeca

Other names: 11-(2-Methylethylidene)1,6-methano[10]annulene
Inchi: InChI=1S/C14H14/c1-11(2)14-12-7-3-4-8-13(14)10-6-5-9-12/h3-10H,1-2H3
InchiKey: HQHJTKCDGOIONO-UHFFFAOYSA-N
Formula: C14H14
SMILES: CC(C)=C1C2=CC=CC=C1C=CC=C2
Mol. weight [g/mol]: 182.26
CAS: 88635-77-2

Physical Properties

Property code	Value	Unit	Source
gf	310.87	kJ/mol	Joback Method
hf	155.39	kJ/mol	Joback Method
hfus	19.99	kJ/mol	Joback Method
hvap	51.71	kJ/mol	Joback Method
ie	7.70	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	-4.59		Crippen Method
logp	3.871		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
tb	576.17	K	Joback Method
tc	817.05	K	Joback Method
tf	299.54	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.12	J/mol×K	576.17	Joback Method
cpg	388.17	J/mol×K	616.32	Joback Method
cpg	403.94	J/mol×K	656.46	Joback Method
cpg	418.53	J/mol×K	696.61	Joback Method
cpg	432.02	J/mol×K	736.76	Joback Method
cpg	444.51	J/mol×K	776.90	Joback Method

cpg	456.08	J/mol×K	817.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88635772&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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