Tetracyclo[4.2.2.22,5.01,6]dodeca-7,9-triene

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

Physical Properties

Property code	Value	Unit	Source
hfus	9.22	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
logp	2.919		Crippen Method
mcvol	127.900	ml/mol	McGowan 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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106697432&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume