Bicyclo[2.2.0]hexa-2,5-diene, 1,2,3,4,5,6-hexamethyl-

Other names: Bicyclo[2.2.0]hexa-2,5-diene, 1,2,3,4,5,6-hexamethyl-
Hexamethyl Dewar benzene
Hexamethylbicyclo[2.2.0]hexa-2,5-diene
1,2,3,4,5,6-Hexamethylbicyclo[2.2.0]hexa-2,5-diene
Bicyclo(2.2.0)hexa-2,5-diene, hexamethyl-
2-Butin hexamethyl-dewar-benzol
Hexamethyl-bicyclo(2.2.0)hexa-2,5-dien
1,2,3,4,5,6-hexamethylbicyclo(2,2,0)hexa-2,5-diene

Inchi: InChI=1S/C12H18/c1-7-8(2)12(6)10(4)9(3)11(7,12)5/h1-6H3

InchiKey: RVNQQZMIWZPGNA-UHFFFAOYSA-N

Formula: C12H18

SMILES: CC1=C(C)C2(C)C(C)=C(C)C12C

Mol. weight [g/mol]: 162.28

Physical Properties

Property code	Value	Unit	Source
chl	-7385.00 ± 4.60	kJ/mol	NIST Webbook
hfl	-90.40	kJ/mol	NIST Webbook
hfus	11.40	kJ/mol	Joback Method
ie	7.83	eV	NIST Webbook
ie	7.92	eV	NIST Webbook
logp	3.699		Crippen Method
mcvol	149.620	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.00	J/mol×K	506.16	Joback Method
cpg	366.37	J/mol×K	541.23	Joback Method
cpg	380.56	J/mol×K	576.29	Joback Method
cpg	393.77	J/mol×K	611.36	Joback Method
cpg	406.21	J/mol×K	646.42	Joback Method
cpg	418.11	J/mol×K	681.49	Joback Method
cpg	429.68	J/mol×K	716.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.20	K	2.70	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7641772&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

hfl: Liquid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tbrp: Boiling point at reduced pressure