Dewar benzene, 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]:	162.27
CAS:	7641-77-2

Physical Properties

Property code	Value	Unit	Source
chl	-7385.00 ± 4.60	kJ/mol	NIST Webbook
gf	182.08	kJ/mol	Joback Method
hf	-45.25	kJ/mol	Joback Method
hfl	-90.40	kJ/mol	NIST Webbook
hfus	11.40	kJ/mol	Joback Method
hvap	43.06	kJ/mol	Joback Method
ie	7.92	eV	NIST Webbook
ie	7.83	eV	NIST Webbook
log10ws	-3.86		Crippen Method
logp	3.699		Crippen Method
mcvol	149.620	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	506.16	K	Joback Method
tc	716.55	K	Joback Method
tf	360.28	K	Joback Method
vc	0.590	m3/kmol	Joback 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

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=C7641772&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume