Hexaphenylmelamine

Inchi: InChI=1S/C39H30N6/c1-7-19-31(20-8-1)43(32-21-9-2-10-22-32)37-40-38(44(33-23-11-3
InchiKey: YGXMMMPUTDCEAF-UHFFFAOYSA-N
Formula: C39H30N6
SMILES: c1ccc(N(c2ccccc2)c2nc(N(c3ccccc3)c3ccccc3)nc(N(c3ccccc3)c3ccccc3)n2)cc1
Mol. weight [g/mol]: 582.70
CAS: 18343-40-3

Physical Properties

Property code	Value	Unit	Source
chs	-20095.00 ± 10.00	kJ/mol	NIST Webbook
hfs	460.00 ± 10.00	kJ/mol	NIST Webbook
log10ws	-11.27		Crippen Method
logp	10.281		Crippen Method
mcvol	453.930	ml/mol	McGowan Method
ss	673.70	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	665.80	J/mol×K	298.15	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18343403&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions