

Hexaphenylisomelamine

Inchi: InChI=1S/C39H30N6/c1-7-19-31(20-8-1)40-37-43(34-25-13-4-14-26-34)38(41-32-21-9-2
InchiKey: MBZKVOZDQXHTIK-UHFFFAOYSA-N
Formula: C39H30N6
SMILES: c1ccc(N=c2n(-c3ccccc3)c(=Nc3ccccc3)n(-c3ccccc3)c(=Nc3ccccc3)n2-c2ccccc2)cc1
Mol. weight [g/mol]: 582.70
CAS: 604-45-5

Physical Properties

Property code	Value	Unit	Source
chs	-20256.00 ± 14.00	kJ/mol	NIST Webbook
hfs	622.00 ± 14.00	kJ/mol	NIST Webbook
log10ws	-10.80		Crippen Method
logp	7.756		Crippen Method
mcvol	453.930	ml/mol	McGowan Method
ss	706.50	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	672.40	J/mol×K	298.15	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C604455&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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