Hexaphenylethane

Inchi: InChI=1S/C38H30/c1-6-16-30(17-7-1)37(31-18-8-2-9-19-31)32-26-28-36(29-27-32)38(33
InchiKey: FWSYACUVHKGULL-UHFFFAOYSA-N
Formula: C38H30
SMILES: C1=CC(C(c2ccccc2)(c2ccccc2)c2ccccc2)C=CC1=C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 486.64
CAS: 18909-18-7

Physical Properties

Property code	Value	Unit	Source
chs	-19920.00	kJ/mol	NIST Webbook
gf	955.25	kJ/mol	Joback Method
hf	582.37	kJ/mol	Joback Method
hfs	674.90	kJ/mol	NIST Webbook
hfus	50.26	kJ/mol	Joback Method
hvap	112.15	kJ/mol	Joback Method
log10ws	-10.60		Crippen Method
logp	9.265		Crippen Method
mcvol	403.720	ml/mol	McGowan Method
pc	1204.80	kPa	Joback Method
tb	1223.40	K	Joback Method
tc	1528.59	K	Joback Method
tf	657.84	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1367.60	J/mol×K	1223.40	Joback Method
cpg	1387.07	J/mol×K	1274.27	Joback Method
cpg	1407.22	J/mol×K	1325.13	Joback Method
cpg	1428.56	J/mol×K	1376.00	Joback Method
cpg	1451.61	J/mol×K	1426.86	Joback Method
cpg	1476.90	J/mol×K	1477.73	Joback Method
cpg	1504.95	J/mol×K	1528.59	Joback Method

hsubt	114.60	kJ/mol	371.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C18909187&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume