2,2',4,4',6,6'-Hexanitrobiphenyl

Inchi: InChI=1S/C12H4N6O12/c19-13(20)5-1-7(15(23)24)11(8(2-5)16(25)26)12-9(17(27)28)3-6

InchiKey: PJTZYMXZEQWUHG-UHFFFAOYSA-N

Formula: C12H4N6O12

SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(-c2c([N+](=O)[O-])cc([N+](=O)[O-])cc2[N+](=O)[O-])c([N

Mol. weight [g/mol]: 424.19

CAS: 4433-16-3

Physical Properties

Property code	Value	Unit	Source
chs	-5362.00 ± 4.00	kJ/mol	NIST Webbook
gf	430.50	kJ/mol	Joback Method
hf	48.67	kJ/mol	Joback Method
hfs	68.20 ± 8.40	kJ/mol	NIST Webbook
hfus	80.75	kJ/mol	Joback Method
hvap	150.38	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	2.803		Crippen Method
mcvol	236.940	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	1468.24	K	Joback Method
tc	1809.37	K	Joback Method
tf	1214.62	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.43	J/mol×K	1468.24	Joback Method
cpg	683.90	J/mol×K	1525.10	Joback Method
cpg	681.96	J/mol×K	1581.95	Joback Method
cpg	679.77	J/mol×K	1638.81	Joback Method
cpg	677.50	J/mol×K	1695.66	Joback Method
cpg	675.32	J/mol×K	1752.52	Joback Method
cpg	673.39	J/mol×K	1809.37	Joback Method

Sources

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=C4433163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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