2,2',4,4',6-Pentanitrobenzophenone

Inchi: InChI=1S/C13H5N5O11/c19-13(8-2-1-6(14(20)21)3-9(8)16(24)25)12-10(17(26)27)4-7(15

InchiKey: SZWQTMLLIXBBNS-UHFFFAOYSA-N

Formula: C13H5N5O11

SMILES: O=C(c1ccc([N+](=O)[O-])cc1[N+](=O)[O-])c1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[

Mol. weight [g/mol]: 407.21

CAS: 32255-35-9

Physical Properties

Property code	Value	Unit	Source
chs	-5716.00 ± 2.00	kJ/mol	NIST Webbook
gf	284.08	kJ/mol	Joback Method
hf	-62.32	kJ/mol	Joback Method
hfs	-115.00 ± 5.00	kJ/mol	NIST Webbook
hfus	73.97	kJ/mol	Joback Method
hvap	142.09	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	2.459		Crippen Method
mcvol	235.180	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	1388.17	K	Joback Method
tc	1714.64	K	Joback Method
tf	1119.69	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.28	J/mol×K	1388.17	Joback Method
cpg	685.00	J/mol×K	1442.58	Joback Method
cpg	684.17	J/mol×K	1496.99	Joback Method
cpg	682.95	J/mol×K	1551.41	Joback Method
cpg	681.50	J/mol×K	1605.82	Joback Method
cpg	679.97	J/mol×K	1660.23	Joback Method
cpg	678.52	J/mol×K	1714.64	Joback Method

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=C32255359&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
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