# N,n',n''-tris(p-nitrophenyl)guanidine

**Inchi:** InChI=1S/C19H14N6O6/c26-23(27)16-7-1-13(2-8-16)20-19(21-14-3-9-17(10-4-14)24(28)
**InchiKey:** CDBWRGOFBAPWQM-UHFFFAOYSA-N
**Formula:** C19H14N6O6
**SMILES:** O=[N+]([O-])c1ccc(N=C(Nc2ccc([N+](=O)[O-])cc2)Nc2ccc([N+](=O)[O-])cc2)cc1
**Mol. weight [g/mol]:** 422.35
**CAS:** 18440-30-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 386.78 | kJ/mol | Joback Method |
| hvap | 132.74 | kJ/mol | Joback Method |
| log10ws | -7.04 | | Crippen Method |
| logp | 4.623 | | Crippen Method |
| mcvol | 285.190 | ml/mol | McGowan Method |
| pc | 2200.01 | kPa | Joback Method |
| tb | 1361.52 | K | Joback Method |
| tc | 1677.23 | K | 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=C18440307&Units=SI

## Legend

**hf:** Enthalpy of formation 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 |