

1,1,3,5-Tetranitrohexahydropyrimidine

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|-----------------------------|--|
| Other names: | 1,3,5,5-Tetranitrohexahydropyrimidine |
| Inchi: | InChI=1S/C4H6N6O8/c11-7(12)4(8(13)14)1-5(9(15)16)3-6(2-4)10(17)18/h1-3H2 |
| InchiKey: | NOEKJIBAIMWJEB-UHFFFAOYSA-N |
| Formula: | C4H6N6O8 |
| SMILES: | O=[N+]([O-])N1CN([N+](=O)[O-])CC([N+](=O)[O-])([N+](=O)[O-])C1 |
| Mol. weight [g/mol]: | 266.13 |
| CAS: | 81360-42-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hfs | 0.40 | kJ/mol | NIST Webbook |
| log10ws | -1.95 | | Crippen Method |
| logp | -1.805 | | Crippen Method |
| mcvol | 146.000 | ml/mol | McGowan Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|--------|-----------------|--------------|
| hfust | 29.37 | kJ/mol | 430.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C81360421&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|-----------------|--|
| hfs: | Solid phase enthalpy of formation at standard conditions |
| hfust: | Enthalpy of fusion at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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