

2-Propanone, (1-methylethylidene)hydrazone

| | |
|-----------------------------|---|
| Other names: | Acetone, azine Acetone ketazine Dimethyl ketazine |
| Inchi: | InChI=1S/C6H12N2/c1-5(2)7-8-6(3)4/h1-4H3 |
| InchiKey: | PFLUPZGCTVGDLV-UHFFFAOYSA-N |
| Formula: | C6H12N2 |
| SMILES: | CC(C)=NN=C(C)C |
| Mol. weight [g/mol]: | 112.17 |
| CAS: | 627-70-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -22.31 | kJ/mol | Joback Method |
| hvap | 35.74 | kJ/mol | Joback Method |
| ie | 7.97 | eV | NIST Webbook |
| ie | 8.60 | eV | NIST Webbook |
| ie | 7.97 | eV | NIST Webbook |
| log10ws | -1.65 | | Crippen Method |
| logp | 1.863 | | Crippen Method |
| mcvol | 106.760 | ml/mol | McGowan Method |
| pc | 2515.07 | kPa | Joback Method |
| rinpol | 828.00 | | NIST Webbook |
| rinpol | 828.00 | | NIST Webbook |
| tb | 406.20 | K | NIST Webbook |
| tc | 706.67 | K | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 406.20 | K | 102.00 | NIST Webbook |
| tbrp | 327.20 | K | 4.90 | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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=C627703&Units=SI |

Legend

| | |
|-----------------|---|
| hf: | Enthalpy of formation at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |

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