

1,2,4-Triazine

| | |
|-----------------------------|--------------------------------------|
| Other names: | as-Triazine |
| Inchi: | InChI=1S/C3H3N3/c1-2-5-6-3-4-1/h1-3H |
| InchiKey: | FYADHXFMURLYQI-UHFFFAOYSA-N |
| Formula: | C3H3N3 |
| SMILES: | c1cnncn1 |
| Mol. weight [g/mol]: | 81.08 |
| CAS: | 290-38-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| ie | 9.20 | eV | NIST Webbook |
| ie | 9.61 | eV | NIST Webbook |
| log10ws | -0.77 | | Crippen Method |
| logp | -0.128 | | Crippen Method |
| mcvol | 59.310 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 429.20 | K | 98.70 | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C290380&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|-------------------------------------|
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| tbrp: | Boiling point at reduced pressure |

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<https://www.chemeo.com/cid/81-269-4/1-2-4-Triazine.pdf>

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