

# Acetic acid, 9h-purine-9-yl-, hydrazide

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C7H8N6O/c8-12-6(14)2-13-4-11-5-1-9-3-10-7(5)13/h1,3-4H,2,8H2,(H,12,14) |
| <b>InchiKey:</b>            | OOOPVODKHFXNEK-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C7H8N6O   |
| <b>SMILES:</b>              | NNC(=O)Cn1cnc2cncnc21   |
| <b>Mol. weight [g/mol]:</b> | 192.18  |
| <b>CAS:</b>                 | 98277-57-7  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.22   |        | Crippen Method |
| logp          | -1.184  |        | Crippen Method |
| mcvol         | 132.020 | ml/mol | McGowan Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C98277577&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C98277577&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |

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