

# 1-Pyrrolidinylacetonitrile

|                      |                                                                                                                                                                       |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1-Pyrrolidineacetonitrile<br>Pyrrolidinoacetonitrile<br>Pyrroldinoacetonitrile<br>1-Cyanomethylpyrrolidine<br>N-Pyrrolidinoacetonitrile<br>pyrrolidine-1-acetonitrile |
| Inchi:               | InChI=1S/C6H10N2/c7-3-6-8-4-1-2-5-8/h1-2,4-6H2                                                                                                                        |
| InchiKey:            | NPRYXVXVLCYBNS-UHFFFAOYSA-N                                                                                                                                           |
| Formula:             | C6H10N2                                                                                                                                                               |
| SMILES:              | N#CCN1CCCC1                                                                                                                                                           |
| Mol. weight [g/mol]: | 110.16                                                                                                                                                                |
| CAS:                 | 29134-29-0                                                                                                                                                            |

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| log10ws       | -0.67  |        | Crippen Method |
| logp          | 0.606  |        | Crippen Method |
| mcvol         | 95.900 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C29134290&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29134290&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |

## Legend

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

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