

# Pyrrolidine, 1-(1-butenyl)-

|                      |                                                                                                                 |
|----------------------|-----------------------------------------------------------------------------------------------------------------|
| Other names:         | 1-(1-Butenyl)pyrrolidine<br>1-(1-Pyrrolidinyl)-1-butene<br>1-Pyrrolidino-1-butene<br>(E)-1-Pyrrolidino-1-butene |
| Inchi:               | InChI=1S/C8H15N/c1-2-3-6-9-7-4-5-8-9/h3,6H,2,4-5,7-8H2,1H3/b6-3+                                                |
| InchiKey:            | GQCQSPFOXSSUEG-ZZXKWWIFSA-N                                                                                     |
| Formula:             | C8H15N                                                                                                          |
| SMILES:              | CCC=CN1CCCC1                                                                                                    |
| Mol. weight [g/mol]: | 125.21                                                                                                          |
| CAS:                 | 13937-89-8                                                                                                      |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| ie            | 6.70    | eV     | NIST Webbook   |
| ie            | 7.24    | eV     | NIST Webbook   |
| log10ws       | -1.98   |        | Crippen Method |
| logp          | 2.006   |        | Crippen Method |
| mcvol         | 118.400 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| 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>                             |
| 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=C13937898&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13937898&amp;Units=SI</a> |

## Legend

|          |                                     |
|----------|-------------------------------------|
| ie:      | Ionization energy                   |
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |

**mcvol:** McGowan's characteristic volume

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