

Pyrrolidine, 1-(2-methyl-1-propenyl)-

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| Other names: | Pyrrolidine, 1-(2-methylpropenyl)- Isobutyraldehyde pyrrolidine enamine N-(2-Methyl-1-propenyl)pyrrolidine N-Isobutenylpyrrolidine 1-(2-Methyl-1-propenyl)pyrrolidine 1-(2-Methylpropenyl)pyrrolidine 1-Pyrrolidino-2-methylpropene 1-Pyrrolidinoisobutene 2-Methyl-1-pyrrolidinopropene |
| Inchi: | InChI=1S/C8H15N/c1-8(2)7-9-5-3-4-6-9/h7H,3-6H2,1-2H3 |
| InchiKey: | PAXNHQZTZQFBPC-UHFFFAOYSA-N |
| Formula: | C8H15N |
| SMILES: | CC(C)=CN1CCCC1 |
| Mol. weight [g/mol]: | 125.21 |
| CAS: | 2403-57-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|--------|----------------|
| ie | 6.80 | eV | NIST Webbook |
| ie | 7.75 | eV | NIST Webbook |
| ie | 7.66 ± 0.03 | eV | NIST Webbook |
| log10ws | -1.98 | | Crippen Method |
| logp | 2.006 | | Crippen Method |
| mvol | 118.400 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2403578&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

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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