

2,5-Pyrrolidinedione, 1-butyl-

| | |
|-----------------------------|---|
| Other names: | Succinimide, N-butyl- n-Butylsuccinimide |
| Inchi: | InChI=1S/C8H13NO2/c1-2-3-6-9-7(10)4-5-8(9)11/h2-6H2,1H3 |
| InchiKey: | HKAIKVVJIRPASO-UHFFFAOYSA-N |
| Formula: | C8H13NO2 |
| SMILES: | CCCCN1C(=O)CCC1=O |
| Mol. weight [g/mol]: | 155.19 |
| CAS: | 3470-96-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.19 | | Crippen Method |
| logp | 0.935 | | Crippen Method |
| mcvol | 125.840 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|---------------|------|----------------|--------------|
| tbrp | 411.00 ± 1.00 | K | 2.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3470960&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

| | |
|-----------------|-------------------------------------|
| 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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