

gly-gly-his

Inchi: InChI=1S/C10H15N5O4/c11-2-8(16)13-4-9(17)15-7(10(18)19)1-6-3-12-5-14-6/h3,5,7H,1
InchiKey: PDAWDNVHMUKWJR-UHFFFAOYSA-N
Formula: C10H15N5O4
SMILES: NCC(=O)NCC(=O)NC(Cc1c[nH]cn1)C(=O)O
Mol. weight [g/mol]: 269.26
CAS: 7451-76-5

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| basg | 979.50 | kJ/mol | NIST Webbook |
| log10ws | 0.07 | | Crippen Method |
| logp | -2.885 | | Crippen Method |
| mcvol | 192.780 | ml/mol | McGowan Method |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7451765&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

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

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