

4,5,6,7-Tetrahydropyrazolo[1,5-d][1,2,4]-triazin-4-one-5-ethyl-2,6-dimethyl

InChI: InChI=1S/C9H16N4O/c1-4-13-9(14)8-5-7(2)10-12(8)6-11(13)3/h8H,4-6H2,1-3H3
InChIKey: UMJPLVHCKVZHMN-UHFFFAOYSA-N
Formula: C9H16N4O
SMILES: CCN1C(=O)C2CC(C)=NN2CN1C
Mol. weight [g/mol]: 196.25

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -0.62 | | Crippen Method |
| logp | 0.103 | | Crippen Method |
| mcvol | 153.140 | ml/mol | McGowan Method |
| rinpole | 2006.00 | | NIST Webbook |

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R582291&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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