

Purine, 6-(p-methoxyphenoxy)-

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H10N4O2/c1-17-8-2-4-9(5-3-8)18-12-10-11(14-6-13-10)15-7-16-12/h2-7H, |
| InchiKey: | KCPNMDHKYFRCCP-UHFFFAOYSA-N |
| Formula: | C12H10N4O2 |
| SMILES: | COc1ccc(Oc2ncnc3nc[nH]c23)cc1 |
| Mol. weight [g/mol]: | 242.23 |
| CAS: | 5446-38-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.55 | | Crippen Method |
| logp | 1.672 | | Crippen Method |
| mcvol | 168.920 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C5446388&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/114-509-0/Purine-6-p-methoxyphenoxy.pdf>

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