

1H-Purin-2-amine, 6-(methylthio)-

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|-----------------------------|---|
| Other names: | Purine, 2-amino-6-(methylthio)- 2-Amino-6-methylmercaptapurine 2-Amino-6-methylthiopurine 6-Methylthioguanine 6-(methylthio)-1H-purin-2-amine |
| Inchi: | InChI=1S/C6H7N5S/c1-12-5-3-4(9-2-8-3)10-6(7)11-5/h2H,1H3,(H3,7,8,9,10,11) |
| InchiKey: | YEGKYFQLKYGHAR-UHFFFAOYSA-N |
| Formula: | C6H7N5S |
| SMILES: | CSc1[nH]c(N)nc2ncnc1-2 |
| Mol. weight [g/mol]: | 181.22 |
| CAS: | 1198-47-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.38 | | Crippen Method |
| logp | 0.127 | | Crippen Method |
| mcvol | 122.730 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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=C1198476&Units=SI |

Legend

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

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