

1H-Purine, 6-methyl-

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|-----------------------------|--|
| Other names: | Purine, 6-methyl- 6-Methylpurine 6-Methyl-1H-purine |
| Inchi: | InChI=1S/C6H6N4/c1-4-5-6(9-2-7-4)10-3-8-5/h2-3H,1H3,(H,7,8,9,10) |
| InchiKey: | SYMHUEFSSMBHJA-UHFFFAOYSA-N |
| Formula: | C6H6N4 |
| SMILES: | Cc1ncnc2[nH]cnc12 |
| Mol. weight [g/mol]: | 134.14 |
| CAS: | 2004-03-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| affp | 939.20 | kJ/mol | NIST Webbook |
| basg | 907.30 | kJ/mol | NIST Webbook |
| ie | 8.90 | eV | NIST Webbook |
| ie | 9.30 | eV | NIST Webbook |
| log10ws | -2.27 | | Crippen Method |
| logp | 0.179 | | Crippen Method |
| mcvol | 96.400 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| 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=C2004037&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|--------------|-----------------|
| affp: | Proton affinity |
| basg: | Gas basicity |

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

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