

5-Acetamido-2-methylphenyl acetate

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|----------------------|---|
| Other names: | 3-Acetyloxy-4-methyl-N-acetylaniline |
| Inchi: | InChI=1S/C11H13NO3/c1-7-4-5-10(12-8(2)13)6-11(7)15-9(3)14/h4-6H,1-3H3,(H,12,13) |
| InchiKey: | BWNMDWQTBHTORP-UHFFFAOYSA-N |
| Formula: | C11H13NO3 |
| SMILES: | CC(=O)Nc1ccc(C)c(OC(C)=O)c1 |
| Mol. weight [g/mol]: | 207.23 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -138.56 | kJ/mol | Joback Method |
| hf | -360.69 | kJ/mol | Joback Method |
| hfus | 26.99 | kJ/mol | Joback Method |
| hvap | 66.02 | kJ/mol | Joback Method |
| log10ws | -2.46 | | Crippen Method |
| logp | 1.879 | | Crippen Method |
| mcvol | 161.080 | ml/mol | McGowan Method |
| pc | 2918.68 | kPa | Joback Method |
| rinpol | 1870.00 | | NIST Webbook |
| tb | 668.05 | K | Joback Method |
| tc | 885.88 | K | Joback Method |
| tf | 439.94 | K | Joback Method |
| vc | 0.609 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 410.21 | J/molxK | 668.05 | Joback Method |
| cpg | 422.70 | J/molxK | 704.36 | Joback Method |
| cpg | 434.40 | J/molxK | 740.66 | Joback Method |
| cpg | 445.32 | J/molxK | 776.97 | Joback Method |
| cpg | 455.45 | J/molxK | 813.27 | Joback Method |
| cpg | 464.82 | J/molxK | 849.58 | Joback Method |
| cpg | 473.43 | J/molxK | 885.88 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373285&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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