

Glucose, 6-ethyl, nitrile, acetylated

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|-----------------------------|--|
| Inchi: | InChI=1S/C16H23NO9/c1-6-22-8-14(24-10(3)19)16(26-12(5)21)15(25-11(4)20)13(7-17)2 |
| InchiKey: | NYLIIOWUKNZONP-ZJIFWQFVSA-N |
| Formula: | C16H23NO9 |
| SMILES: | CCOCC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(C#N)OC(C)=O |
| Mol. weight [g/mol]: | 373.36 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| gf | -833.42 | kJ/mol | Joback Method |
| hf | -1341.23 | kJ/mol | Joback Method |
| hfus | 36.95 | kJ/mol | Joback Method |
| hvap | 99.17 | kJ/mol | Joback Method |
| log10ws | -1.37 | | Crippen Method |
| logp | 0.273 | | Crippen Method |
| mcvol | 273.310 | ml/mol | McGowan Method |
| pc | 1502.31 | kPa | Joback Method |
| rinpol | 2024.00 | | NIST Webbook |
| rinpol | 2018.00 | | NIST Webbook |
| rinpol | 2014.00 | | NIST Webbook |
| rinpol | 2024.00 | | NIST Webbook |
| tb | 993.38 | K | Joback Method |
| tc | 1216.96 | K | Joback Method |
| tf | 585.94 | K | Joback Method |
| vc | 1.048 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 870.38 | J/molxK | 993.38 | Joback Method |
| cpg | 878.74 | J/molxK | 1030.64 | Joback Method |
| cpg | 885.36 | J/molxK | 1067.91 | Joback Method |
| cpg | 890.18 | J/molxK | 1105.17 | Joback Method |
| cpg | 893.17 | J/molxK | 1142.44 | Joback Method |
| cpg | 894.29 | J/molxK | 1179.70 | 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=R530319&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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/36-382-8/Glucose-6-ethyl-nitrile-acetylated.pdf>

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