# Hydratropic acid, 2-methyloct-5-yn-4-yl ester

**Inchi:** InChI=1S/C18H24O2/c1-5-6-12-17(13-14(2)3)20-18(19)15(4)16-10-8-7-9-11-16/h7-11,14
**InchiKey:** HXVNSFXUARBLNQ-UHFFFAOYSA-N
**Formula:** C18H24O2
**SMILES:** CCC#CC(CC(C)C)OC(=O)C(C)c1ccccc1
**Mol. weight [g/mol]:** 272.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 174.65 | kJ/mol | Joback Method |
| hf | -166.66 | kJ/mol | Joback Method |
| hfus | 31.76 | kJ/mol | Joback Method |
| hvap | 68.08 | kJ/mol | Joback Method |
| log10ws | -4.95 | | Crippen Method |
| logp | 4.161 | | Crippen Method |
| mcvol | 239.560 | ml/mol | McGowan Method |
| pc | 1758.02 | kPa | Joback Method |
| rinpol | 1793.00 | | NIST Webbook |
| rinpol | 1793.00 | | NIST Webbook |
| tb | 721.89 | K | Joback Method |
| tc | 942.19 | K | Joback Method |
| tf | 452.30 | K | Joback Method |
| vc | 0.903 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 667.00 | J/mol×K | 721.89 | Joback Method |
| cpg | 685.32 | J/mol×K | 758.61 | Joback Method |
| cpg | 702.43 | J/mol×K | 795.32 | Joback Method |
| cpg | 718.36 | J/mol×K | 832.04 | Joback Method |
| cpg | 733.16 | J/mol×K | 868.76 | Joback Method |
| cpg | 746.87 | J/mol×K | 905.48 | Joback Method |
| cpg | 759.53 | J/mol×K | 942.19 | Joback Method |

# Sources

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|---|---|
| **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=U406958&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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