# Hexanoic acid, 2-phenylethyl ester

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|---|---|
| **Other names:** | 2-Phenethyl hexanoate |
| | 2-phenylethyl caproate |
| | 2-phenylethyl hexanoate |
| | Hexanoic acid, phenethyl ester |
| | NSC 6651 |
| | Phenylethyl caproate |
| | Phenylethyl hexanoate |
| | Phenylethyl n-hexanoate |
| | phenethyl hexanoate |
| **Inchi:** | InChI=1S/C14H20O2/c1-2-3-5-10-14(15)16-12-11-13-8-6-4-7-9-13/h4,6-9H,2-3,5,10-12H |
| **InchiKey:** | BUYNWUMUDHPPDS-UHFFFAOYSA-N |
| **Formula:** | C14H20O2 |
| **SMILES:** | CCCCCC(=O)OCCc1ccccc1 |
| **Mol. weight [g/mol]:** | 220.31 |
| **CAS:** | 6290-37-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -54.51 | kJ/mol | Joback Method |
| hf | -340.56 | kJ/mol | Joback Method |
| hfus | 28.84 | kJ/mol | Joback Method |
| hvap | 58.19 | kJ/mol | Joback Method |
| log10ws | -3.65 | | Crippen Method |
| logp | 3.353 | | Crippen Method |
| mcvol | 191.800 | ml/mol | McGowan Method |
| pc | 2094.58 | kPa | Joback Method |
| rinpol | 1616.00 | | NIST Webbook |
| rinpol | 1613.00 | | NIST Webbook |
| rinpol | 1619.00 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1643.00 | | NIST Webbook |
| rinpol | 1660.00 | | NIST Webbook |
| rinpol | 1657.00 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1618.00 | | NIST Webbook |
| rinpol | 1618.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1649.00 | | NIST Webbook |
| rinpol | 1606.00 | | NIST Webbook |
| rinpol | 1639.00 | | NIST Webbook |
| rinpol | 1645.60 | | NIST Webbook |
| rinpol | 1650.00 | | NIST Webbook |
| rinpol | 1642.00 | | NIST Webbook |
| ripol | 2165.00 | | NIST Webbook |
| ripol | 2178.00 | | NIST Webbook |
| ripol | 2134.00 | | NIST Webbook |
| ripol | 2134.00 | | NIST Webbook |
| ripol | 2136.00 | | NIST Webbook |
| ripol | 2164.00 | | NIST Webbook |
| ripol | 2166.00 | | NIST Webbook |
| ripol | 2160.00 | | NIST Webbook |
| ripol | 2160.00 | | NIST Webbook |
| ripol | 2165.00 | | NIST Webbook |
| tb | 622.69 | K | Joback Method |
| tc | 822.76 | K | Joback Method |
| tf | 346.12 | K | Joback Method |
| vc | 0.736 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 579.01 | J/mol×K | 822.76 | Joback Method |
| cpg | 494.13 | J/mol×K | 622.69 | Joback Method |
| cpg | 510.47 | J/mol×K | 656.04 | Joback Method |
| cpg | 525.89 | J/mol×K | 689.38 | Joback Method |
| cpg | 540.43 | J/mol×K | 722.73 | Joback Method |
| cpg | 554.11 | J/mol×K | 756.07 | Joback Method |
| cpg | 566.96 | J/mol×K | 789.42 | Joback Method |
| dvisc | 0.0001517 | Pa×s | 622.69 | Joback Method |
| dvisc | 0.0020543 | Pa×s | 346.12 | Joback Method |
| dvisc | 0.0010310 | Pa×s | 392.21 | Joback Method |
| dvisc | 0.0005982 | Pa×s | 438.31 | Joback Method |
| dvisc | 0.0003849 | Pa×s | 484.40 | Joback Method |
| dvisc | 0.0002674 | Pa×s | 530.50 | Joback Method |
| dvisc | 0.0001969 | Pa×s | 576.60 | Joback Method |

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|---|---|---|---|---|
| hvapt | 78.80 | kJ/mol | 298.15 | Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography |

# 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=C6290375&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:** | https://www.doi.org/10.1016/j.jct.2015.02.015 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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