# Lavandulyl butyrate

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|---|---|
| **Inchi:** | InChI=1S/C14H24O2/c1-6-7-14(15)16-10-13(12(4)5)9-8-11(2)3/h8,13H,4,6-7,9-10H2,1-3 |
| **InchiKey:** | ROJSUZRYGHOLJL-UHFFFAOYSA-N |
| **Formula:** | C14H24O2 |
| **SMILES:** | C=C(C)C(CC=C(C)C)COC(=O)CCC |
| **Mol. weight [g/mol]:** | 224.34 |
| **CAS:** | 59550-35-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -18.40 | kJ/mol | Joback Method |
| hf | -359.30 | kJ/mol | Joback Method |
| hfus | 27.58 | kJ/mol | Joback Method |
| hvap | 54.97 | kJ/mol | Joback Method |
| log10ws | -4.01 | | Crippen Method |
| logp | 3.878 | | Crippen Method |
| mcvol | 206.960 | ml/mol | McGowan Method |
| pc | 1730.34 | kPa | Joback Method |
| rinpol | 1459.70 | | NIST Webbook |
| rinpol | 1459.70 | | NIST Webbook |
| tb | 596.17 | K | Joback Method |
| tc | 781.23 | K | Joback Method |
| tf | 269.94 | K | Joback Method |
| vc | 0.800 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 525.99 | J/mol×K | 596.17 | Joback Method |
| cpg | 542.76 | J/mol×K | 627.01 | Joback Method |
| cpg | 558.71 | J/mol×K | 657.86 | Joback Method |
| cpg | 573.90 | J/mol×K | 688.70 | Joback Method |
| cpg | 588.33 | J/mol×K | 719.54 | Joback Method |
| cpg | 602.04 | J/mol×K | 750.38 | Joback Method |
| cpg | 615.07 | J/mol×K | 781.23 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C59550355&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# 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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