# 8,9-Dehydrothymyl isobutyrate

**Inchi:** InChI=1S/C14H18O2/c1-9(2)12-7-6-11(5)8-13(12)16-14(15)10(3)4/h6-8,10H,1H2,2-5H3
**InchiKey:** BSAPRZRKFYAPEB-UHFFFAOYSA-N
**Formula:** C14H18O2
**SMILES:** C=C(C)c1ccc(C)cc1OC(=O)C(C)C
**Mol. weight [g/mol]:** 218.29
**CAS:** 38146-79-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 3.08 | kJ/mol | Joback Method |
| hf | -253.14 | kJ/mol | Joback Method |
| hfus | 21.95 | kJ/mol | Joback Method |
| hvap | 58.54 | kJ/mol | Joback Method |
| log10ws | -4.10 | | Crippen Method |
| logp | 3.590 | | Crippen Method |
| mcvol | 187.500 | ml/mol | McGowan Method |
| pc | 2143.35 | kPa | Joback Method |
| rinpol | 1454.00 | | NIST Webbook |
| rinpol | 1479.10 | | NIST Webbook |
| ripol | 1922.00 | | NIST Webbook |
| tb | 628.77 | K | Joback Method |
| tc | 841.84 | K | Joback Method |
| tf | 340.44 | K | Joback Method |
| vc | 0.712 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 471.75 | J/mol×K | 628.77 | Joback Method |
| cpg | 487.67 | J/mol×K | 664.28 | Joback Method |
| cpg | 502.68 | J/mol×K | 699.79 | Joback Method |
| cpg | 516.80 | J/mol×K | 735.31 | Joback Method |
| cpg | 530.05 | J/mol×K | 770.82 | Joback Method |
| cpg | 542.46 | J/mol×K | 806.33 | Joback Method |

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|---|---|---|---|---|
| cpg | 554.04 | J/mol×K | 841.84 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C38146791&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

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

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