# (3S,3aR)-3-Butyl-3a,4,5,6-tetrahydroisobenzofuran

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|---|---|
| **Other names:** | (3S,3aR)-(-)-Sedanolide<br>trans-Sedanolide<br>trans-Neocnidilide<br>Sedanolide, trans-<br>1(3H)-Isobenzofuranone, 3-butyl-3a,4,5,6-tetrahydro-, (3S,3aR)-<br>Neocnidilide |
| **Inchi:** | InChI=1S/C12H18O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h7,9,11H,2-6,8H2,1H3/t9- |
| **InchiKey:** | UPJFTVFLSIQQAV-GXSJLCMTSA-N |
| **Formula:** | C12H18O2 |
| **SMILES:** | CCCCC1OC(=O)C2=CCCCC21 |
| **Mol. weight [g/mol]:** | 194.27 |
| **CAS:** | 4567-33-3 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -53.02 | kJ/mol | Joback Method |
| hf | -387.28 | kJ/mol | Joback Method |
| hfus | 25.13 | kJ/mol | Joback Method |
| hvap | 52.36 | kJ/mol | Joback Method |
| log10ws | -3.22 | | Crippen Method |
| logp | 2.828 | | Crippen Method |
| mcvol | 161.360 | ml/mol | McGowan Method |
| pc | 2530.27 | kPa | Joback Method |
| rinpol | 1735.00 | | NIST Webbook |
| tb | 599.16 | K | Joback Method |
| tc | 822.08 | K | Joback Method |
| tf | 358.39 | K | Joback Method |
| vc | 0.612 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 437.41 | J/mol×K | 599.16 | Joback Method |
| cpg | 456.37 | J/mol×K | 636.31 | Joback Method |

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|---|---|---|---|---|
| cpg | 474.21 | J/mol×K | 673.47 | Joback Method |
| cpg | 490.96 | J/mol×K | 710.62 | Joback Method |
| cpg | 506.65 | J/mol×K | 747.77 | Joback Method |
| cpg | 521.32 | J/mol×K | 784.93 | Joback Method |
| cpg | 534.98 | J/mol×K | 822.08 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4567333&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 |

# 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 |