

# 8,9,10-trinorborn-5-ene-2-spiro-1'-(2'-butyroxycyc

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C16H24O2/c1-2-5-15(17)18-14-6-3-4-9-16(14)11-12-7-8-13(16)10-12/h7-8,12- |
| <b>InchiKey:</b>            | NGCMNMVPUGHUJL-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C16H24O2  |
| <b>SMILES:</b>              | CCCC(=O)OC1CCCCC12CC1C=CC2C1  |
| <b>Mol. weight [g/mol]:</b> | 248.36  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 12.63   | kJ/mol               | Joback Method  |
| hf            | -365.77 | kJ/mol               | Joback Method  |
| hfus          | 24.08   | kJ/mol               | Joback Method  |
| hvap          | 59.45   | kJ/mol               | Joback Method  |
| log10ws       | -4.31   |                      | Crippen Method |
| logp          | 3.855   |                      | Crippen Method |
| mvol          | 206.860 | ml/mol               | McGowan Method |
| pc            | 2075.54 | kPa                  | Joback Method  |
| ripol         | 1757.00 |                      | NIST Webbook   |
| ripol         | 2214.30 |                      | NIST Webbook   |
| tb            | 669.53  | K                    | Joback Method  |
| tc            | 892.79  | K                    | Joback Method  |
| tf            | 405.92  | K                    | Joback Method  |
| vc            | 0.785   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 618.08 | J/mol×K | 669.53          | Joback Method |
| cpg           | 639.34 | J/mol×K | 706.74          | Joback Method |
| cpg           | 659.40 | J/mol×K | 743.95          | Joback Method |
| cpg           | 678.44 | J/mol×K | 781.16          | Joback Method |
| cpg           | 696.64 | J/mol×K | 818.37          | Joback Method |
| cpg           | 714.19 | J/mol×K | 855.58          | Joback Method |
| cpg           | 731.27 | J/mol×K | 892.79          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R327787&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R327787&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |

# Legend

|                  |   |
|------------------|---|
| <b>cpg:</b>      | Ideal gas heat capacity                         |
| <b>gf:</b>       | Standard Gibbs free energy of formation         |
| <b>hf:</b>       | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>     | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>     | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b>  | Log10 of Water solubility in mol/l              |
| <b>logp:</b>     | Octanol/Water partition coefficient             |
| <b>mcvol:</b>    | McGowan's characteristic volume                 |
| <b>pc:</b>       | Critical Pressure                               |
| <b>rinpolar:</b> | Non-polar retention indices                     |
| <b>ripolar:</b>  | Polar retention indices                         |
| <b>tb:</b>       | Normal Boiling Point Temperature                |
| <b>tc:</b>       | Critical Temperature                            |
| <b>tf:</b>       | Normal melting (fusion) point                   |
| <b>vc:</b>       | Critical Volume                                 |

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