

# Dihydroedulan ia

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C13H22O/c1-10-6-7-11-12(2,3)8-5-9-13(11,4)14-10/h5,9-11H,6-8H2,1-4H3/t10 |
| InchiKey:            | IVTQSEFLDHBCDZ-XEEJXUNPSA-N                                                       |
| Formula:             | C13H22O                                                                           |
| SMILES:              | C[C@H]1CCC2C(C)(C)CC=C[C@@]2(C)O1                                                 |
| Mol. weight [g/mol]: | 194.32                                                                            |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hfus          | 16.04   | kJ/mol | Joback Method  |
| logp          | 3.546   |        | Crippen Method |
| mcvol         | 173.880 | ml/mol | McGowan Method |
| rinpol        | 1292.00 |        | NIST Webbook   |
| rinpol        | 1292.00 |        | NIST Webbook   |
| rinpol        | 1292.00 |        | NIST Webbook   |
| rinpol        | 1293.00 |        | NIST Webbook   |
| rinpol        | 1292.00 |        | NIST Webbook   |
| rinpol        | 1293.00 |        | NIST Webbook   |
| rinpol        | 1293.00 |        | NIST Webbook   |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 451.15 | J/mol×K | 544.65          | Joback Method |
| cpg           | 473.87 |         | 582.97          | Joback Method |
| cpg           | 494.99 |         | 621.29          | Joback Method |
| cpg           | 514.78 |         | 659.61          | Joback Method |
| cpg           | 533.50 |         | 697.93          | Joback Method |
| cpg           | 551.39 |         | 736.24          | Joback Method |
| cpg           | 568.71 |         | 774.56          | Joback Method |

## Sources

|                                  |                                                                                                                                               |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b>           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>Crippen Method:</b>           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>Cheméo Relay (1.0):</b>       |                                                                                                                                               |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                               |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C74006614&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C74006614&amp;Units=SI</a> |
| <b>Joback Method:</b>            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |

## Legend

|                 |                                           |
|-----------------|-------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                   |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions |
| <b>logp:</b>    | Octanol/Water partition coefficient       |
| <b>mcvol:</b>   | McGowan's characteristic volume           |
| <b>rinpola:</b> | Non-polar retention indices               |

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