

# Isophthalic acid, 1-adamantylmethyl heptyl ester

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C26H36O4/c1-2-3-4-5-6-10-29-24(27)22-8-7-9-23(14-22)25(28)30-18-26-15-19 |
| InchiKey:            | XNOIWDXCNVECIU-UHFFFAOYSA-N   |
| Formula:             | C26H36O4  |
| SMILES:              | CCCCCCCOC(=O)c1cccc(C(=O)OCC23CC4CC(CC(C4)C2)C3)c1                                |
| Mol. weight [g/mol]: | 412.56  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -40.07  | kJ/mol               | Joback Method  |
| hf            | -637.37 | kJ/mol               | Joback Method  |
| hfus          | 49.40   | kJ/mol               | Joback Method  |
| hvap          | 93.17   | kJ/mol               | Joback Method  |
| log10ws       | -7.37   |                      | Crippen Method |
| logp          | 6.187   |                      | Crippen Method |
| mvol          | 335.740 | ml/mol               | McGowan Method |
| pc            | 1206.47 | kPa                  | Joback Method  |
| rinpol        | 3350.00 |                      | NIST Webbook   |
| rinpol        | 3350.00 |                      | NIST Webbook   |
| tb            | 998.58  | K                    | Joback Method  |
| tc            | 1228.76 | K                    | Joback Method  |
| tf            | 636.00  | K                    | Joback Method  |
| vc            | 1.292   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1208.27 | J/mol×K | 998.58          | Joback Method |
| cpg           | 1231.81 | J/mol×K | 1036.94         | Joback Method |
| cpg           | 1255.41 | J/mol×K | 1075.31         | Joback Method |
| cpg           | 1279.29 | J/mol×K | 1113.67         | Joback Method |
| cpg           | 1303.72 | J/mol×K | 1152.03         | Joback Method |
| cpg           | 1328.91 | J/mol×K | 1190.40         | Joback Method |
| cpg           | 1355.13 | J/mol×K | 1228.76         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U343967&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343967&amp;Units=SI</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>hvp:</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>rinp:</b>    | Non-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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