

# Succinic acid, 2-biphenyl 4-isopropylphenyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C25H24O4/c1-18(2)19-12-14-21(15-13-19)28-24(26)16-17-25(27)29-23-11-7-6 |
| <b>InchiKey:</b>            | HJIPHGJEEOEUCV-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C25H24O4   |
| <b>SMILES:</b>              | CC(C)c1ccc(OC(=O)CCC(=O)Oc2ccccc2-c2ccccc2)cc1                                   |
| <b>Mol. weight [g/mol]:</b> | 388.46   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 7.31    | kJ/mol               | Joback Method  |
| hf            | -367.56 | kJ/mol               | Joback Method  |
| hfus          | 43.90   | kJ/mol               | Joback Method  |
| hvap          | 97.32   | kJ/mol               | Joback Method  |
| log10ws       | -7.54   |                      | Crippen Method |
| logp          | 5.768   |                      | Crippen Method |
| mvol          | 306.710 | ml/mol               | McGowan Method |
| pc            | 1531.86 | kPa                  | Joback Method  |
| rinpol        | 3074.00 |                      | NIST Webbook   |
| rinpol        | 3074.00 |                      | NIST Webbook   |
| tb            | 1013.54 | K                    | Joback Method  |
| tc            | 1260.35 | K                    | Joback Method  |
| tf            | 605.13  | K                    | Joback Method  |
| vc            | 1.153   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 967.29    | J/molxK | 1013.54         | Joback Method |
| cpg           | 979.21    | J/molxK | 1054.68         | Joback Method |
| cpg           | 989.59    | J/molxK | 1095.81         | Joback Method |
| cpg           | 998.50    | J/molxK | 1136.95         | Joback Method |
| cpg           | 1006.04   | J/molxK | 1178.08         | Joback Method |
| cpg           | 1012.26   | J/molxK | 1219.22         | Joback Method |
| cpg           | 1017.25   | J/molxK | 1260.35         | Joback Method |
| dvisc         | 0.0002618 | Paxs    | 605.13          | Joback Method |

|       |           |      |         |               |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0001475 | Paxs | 673.20  | Joback Method |
| dvisc | 0.0000923 | Paxs | 741.27  | Joback Method |
| dvisc | 0.0000625 | Paxs | 809.34  | Joback Method |
| dvisc | 0.0000449 | Paxs | 877.40  | Joback Method |
| dvisc | 0.0000339 | Paxs | 945.47  | Joback Method |
| dvisc | 0.0000266 | Paxs | 1013.54 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=U360723&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360723&amp;Units=SI</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>                                 |

## Legend

|                                       |   |
|---------------------------------------|---|
| <b>cp<sub>g</sub>:</b>                | Ideal gas heat capacity                         |
| <b>dvisc:</b>                         | Dynamic viscosity                               |
| <b>g<sub>f</sub>:</b>                 | Standard Gibbs free energy of formation         |
| <b>h<sub>f</sub>:</b>                 | Enthalpy of formation at standard conditions    |
| <b>h<sub>fus</sub>:</b>               | Enthalpy of fusion at standard conditions       |
| <b>h<sub>vap</sub>:</b>               | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>w<sub>s</sub>:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</b>               | Octanol/Water partition coefficient             |
| <b>mc<sub>vol</sub>:</b>              | McGowan's characteristic volume                 |
| <b>pc:</b>                            | Critical Pressure                               |
| <b>rin<sub>pol</sub>:</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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