

# Glutaric acid, 2-ethylphenyl hexadecyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C29H48O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-19-25-32-28(30)23-20-24-29 |
| <b>InchiKey:</b>            | NUVCGZWTJYPLMG-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C29H48O4   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1CC  |
| <b>Mol. weight [g/mol]:</b> | 460.69   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -171.76 | kJ/mol               | Joback Method  |
| hf            | -906.43 | kJ/mol               | Joback Method  |
| hfus          | 70.09   | kJ/mol               | Joback Method  |
| hvap          | 101.40  | kJ/mol               | Joback Method  |
| log10ws       | -9.40   |                      | Crippen Method |
| logp          | 8.349   |                      | Crippen Method |
| mvol          | 410.590 | ml/mol               | McGowan Method |
| pc            | 774.18  | kPa                  | Joback Method  |
| rinpol        | 3414.00 |                      | NIST Webbook   |
| rinpol        | 3414.00 |                      | NIST Webbook   |
| tb            | 1047.16 | K                    | Joback Method  |
| tc            | 1291.10 | K                    | Joback Method  |
| tf            | 599.85  | K                    | Joback Method  |
| vc            | 1.599   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1433.07   | J/molxK | 1047.16         | Joback Method |
| cpg           | 1451.70   | J/molxK | 1087.82         | Joback Method |
| cpg           | 1468.40   | J/molxK | 1128.47         | Joback Method |
| cpg           | 1483.25   | J/molxK | 1169.13         | Joback Method |
| cpg           | 1496.34   | J/molxK | 1209.79         | Joback Method |
| cpg           | 1507.75   | J/molxK | 1250.44         | Joback Method |
| cpg           | 1517.56   | J/molxK | 1291.10         | Joback Method |
| dvisc         | 0.0002083 | Paxs    | 599.85          | Joback Method |

|       |           |      |         |               |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0001042 | Paxs | 674.40  | Joback Method |
| dvisc | 0.0000598 | Paxs | 748.95  | Joback Method |
| dvisc | 0.0000380 | Paxs | 823.50  | Joback Method |
| dvisc | 0.0000260 | Paxs | 898.06  | Joback Method |
| dvisc | 0.0000189 | Paxs | 972.61  | Joback Method |
| dvisc | 0.0000143 | Paxs | 1047.16 | 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=U358516&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358516&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>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>rinpol:</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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