

# Sebacic acid, 2,4-dichlorophenethyl hexyl ester

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C24H36Cl2O4/c1-2-3-4-11-17-29-23(27)12-9-7-5-6-8-10-13-24(28)30-18-16-20 |
| InchiKey:            | XFAZQPPJNCKUJM-UHFFFAOYSA-N   |
| Formula:             | C24H36Cl2O4   |
| SMILES:              | CCCCCOC(=O)CCCCCCCC(=O)OCCc1ccc(Cl)cc1Cl  |
| Mol. weight [g/mol]: | 459.45  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -247.35 | kJ/mol               | Joback Method  |
| hf            | -846.18 | kJ/mol               | Joback Method  |
| hfus          | 65.15   | kJ/mol               | Joback Method  |
| hvap          | 99.70   | kJ/mol               | Joback Method  |
| log10ws       | -8.07   |                      | Crippen Method |
| logp          | 7.323   |                      | Crippen Method |
| mvol          | 364.620 | ml/mol               | McGowan Method |
| pc            | 974.73  | kPa                  | Joback Method  |
| rinpol        | 3059.00 |                      | NIST Webbook   |
| rinpol        | 3059.00 |                      | NIST Webbook   |
| tb            | 1012.60 | K                    | Joback Method  |
| tc            | 1239.97 | K                    | Joback Method  |
| tf            | 615.86  | K                    | Joback Method  |
| vc            | 1.417   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1169.66   | J/molxK | 1012.60         | Joback Method |
| cpg           | 1184.22   | J/molxK | 1050.50         | Joback Method |
| cpg           | 1197.29   | J/molxK | 1088.39         | Joback Method |
| cpg           | 1208.93   | J/molxK | 1126.29         | Joback Method |
| cpg           | 1219.16   | J/molxK | 1164.18         | Joback Method |
| cpg           | 1228.05   | J/molxK | 1202.08         | Joback Method |
| cpg           | 1235.63   | J/molxK | 1239.97         | Joback Method |
| dvisc         | 0.0002177 | Paxs    | 615.86          | Joback Method |

|       |           |      |         |               |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0001239 | Paxs | 681.98  | Joback Method |
| dvisc | 0.0000779 | Paxs | 748.11  | Joback Method |
| dvisc | 0.0000528 | Paxs | 814.23  | Joback Method |
| dvisc | 0.0000380 | Paxs | 880.35  | Joback Method |
| dvisc | 0.0000286 | Paxs | 946.48  | Joback Method |
| dvisc | 0.0000223 | Paxs | 1012.60 | 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>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416820&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416820&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>                                     |

## 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>mccvol:</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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