

# Adipic acid, dec-4-enyl heptyl ester

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C23H42O4/c1-3-5-7-9-10-11-13-17-21-27-23(25)19-15-14-18-22(24)26-20-16- |
| InchiKey:            | MFYIPVBLPCLIT-ZHACJKMWSA-N                                                       |
| Formula:             | C23H42O4                                                                         |
| SMILES:              | CCCCC=CCCCOC(=O)CCCCC(=O)OCCCCCCC                                                |
| Mol. weight [g/mol]: | 382.58                                                                           |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -244.84 | kJ/mol  | Joback Method  |
| hf            | -890.43 | kJ/mol  | Joback Method  |
| hfus          | 61.10   | kJ/mol  | Joback Method  |
| hvap          | 85.06   | kJ/mol  | Joback Method  |
| log10ws       | -7.03   |         | Crippen Method |
| logp          | 6.520   |         | Crippen Method |
| mcvol         | 345.510 | ml/mol  | McGowan Method |
| pc            | 928.37  | kPa     | Joback Method  |
| rinpol        | 2617.00 |         | NIST Webbook   |
| rinpol        | 2617.00 |         | NIST Webbook   |
| tb            | 882.38  | K       | Joback Method  |
| tc            | 1080.29 | K       | Joback Method  |
| tf            | 488.21  | K       | Joback Method  |
| vc            | 1.351   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1127.87   | J/mol×K | 882.38          | Joback Method |
| cpg           | 1146.91   | J/mol×K | 915.36          | Joback Method |
| cpg           | 1164.75   | J/mol×K | 948.35          | Joback Method |
| cpg           | 1181.44   | J/mol×K | 981.33          | Joback Method |
| cpg           | 1197.00   | J/mol×K | 1014.32         | Joback Method |
| cpg           | 1211.47   | J/mol×K | 1047.30         | Joback Method |
| cpg           | 1224.91   | J/mol×K | 1080.29         | Joback Method |
| dvisc         | 0.0005530 | Pa×s    | 488.21          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002548 | Pa×s | 553.90 | Joback Method |
| dvisc | 0.0001384 | Pa×s | 619.60 | Joback Method |
| dvisc | 0.0000845 | Pa×s | 685.30 | Joback Method |
| dvisc | 0.0000562 | Pa×s | 750.99 | Joback Method |
| dvisc | 0.0000400 | Pa×s | 816.68 | Joback Method |
| dvisc | 0.0000299 | Pa×s | 882.38 | 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=U354142&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354142&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>                                 |
| <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>                                     |

## 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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