# Adipic acid, decyl octyl ester

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|---|---|
| **Other names:** | Hexanedioic acid, decyl octyl ester |
| | Adipic acid, decyl octyl ester |
| | Octyl decyl adipate |
| **Inchi:** | InChI=1S/C24H46O4/c1-3-5-7-9-11-12-14-18-22-28-24(26)20-16-15-19-23(25)27-21-17- |
| **InchiKey:** | NWSGBTCJMJADLE-UHFFFAOYSA-N |
| **Formula:** | C24H46O4 |
| **SMILES:** | CCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCC |
| **Mol. weight [g/mol]:** | 398.63 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 1.1915 | | Cheméo Relay (1.0) |
| hf | -1148.66 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 63.49 | kJ/mol | Joback Method |
| hvap | 114.40 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.56 | eV | Cheméo Relay (1.0) |
| log10ws | -6.46 | | Cheméo Relay (1.0) |
| logp | 7.134 | | Crippen Method |
| mcvol | 363.900 | ml/mol | McGowan Method |
| pc | 849.99 | kPa | Joback Method |
| rinpol | 2745.00 | | NIST Webbook |
| rinpol | 2745.00 | | NIST Webbook |
| rinpol | 2745.00 | | NIST Webbook |
| tb | 639.00 | K | Cheméo Relay (1.0) |
| tc | 811.76 | K | Cheméo Relay (1.0) |
| tf | 295.35 | K | Cheméo Relay (1.0) |
| vc | 1.425 | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1217.58 | J/mol×K | 901.10 | Joback Method |
| cpg | 1237.78 | J/mol×K | 935.03 | Joback Method |
| cpg | 1256.57 | J/mol×K | 968.97 | Joback Method |

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|---|---|---|---|---|
| cpg | 1273.99 | J/mol×K | 1002.90 | Joback Method |
| cpg | 1290.07 | J/mol×K | 1036.83 | Joback Method |
| cpg | 1304.84 | J/mol×K | 1070.77 | Joback Method |
| cpg | 1318.35 | J/mol×K | 1104.70 | Joback Method |
| dvisc | 0.0005261 | Pa×s | 504.56 | Joback Method |
| dvisc | 0.0002463 | Pa×s | 570.65 | Joback Method |
| dvisc | 0.0001350 | Pa×s | 636.74 | Joback Method |
| dvisc | 0.0000828 | Pa×s | 702.83 | Joback Method |
| dvisc | 0.0000553 | Pa×s | 768.92 | Joback Method |
| dvisc | 0.0000393 | Pa×s | 835.01 | Joback Method |
| dvisc | 0.0000294 | Pa×s | 901.10 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C110292&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**

# Legend

**af:** Acentric Factor
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**rinpol:** Non-polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature

| | |
|---|---|
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |