# DL-2,3-Dimethoxy-2,3-diphenylsuccinonitrile

**Inchi:** InChI=1S/C18H16N2O2/c1-21-17(13-19,15-9-5-3-6-10-15)18(14-20,22-2)16-11-7-4-8-12
**InchiKey:** IESMRPVAAQUHSX-UHFFFAOYSA-N
**Formula:** C18H16N2O2
**SMILES:** COC(C#N)(c1ccccc1)C(C#N)(OC)c1ccccc1
**Mol. weight [g/mol]:** 292.33
**CAS:** 61502-57-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 387.54 | kJ/mol | Joback Method |
| hf | 175.00 | kJ/mol | NIST Webbook |
| hfus | 21.02 | kJ/mol | Joback Method |
| hvap | 83.40 | kJ/mol | Joback Method |
| log10ws | -3.81 | | Crippen Method |
| logp | 3.117 | | Crippen Method |
| mcvol | 231.460 | ml/mol | McGowan Method |
| pc | 1841.99 | kPa | Joback Method |
| tb | 907.14 | K | Joback Method |
| tc | 1166.29 | K | Joback Method |
| tf | 524.74 | K | Joback Method |
| vc | 0.893 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 680.74 | J/mol×K | 907.14 | Joback Method |
| cpg | 692.09 | J/mol×K | 950.33 | Joback Method |
| cpg | 702.36 | J/mol×K | 993.52 | Joback Method |
| cpg | 711.67 | J/mol×K | 1036.71 | Joback Method |
| cpg | 720.16 | J/mol×K | 1079.91 | Joback Method |
| cpg | 727.96 | J/mol×K | 1123.10 | Joback Method |
| cpg | 735.20 | J/mol×K | 1166.29 | Joback Method |
| cps | 305.80 | J/mol×K | 298.15 | NIST Webbook |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C61502576&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **cps:** | Solid phase heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |