

# Diethyl 2-(2-cyanoethyl)-malonate

|                      |                                                                                                                |
|----------------------|----------------------------------------------------------------------------------------------------------------|
| Other names:         | Diethyl (2-cyanoethyl)malonate<br>Propanedioic acid, (2-cyanoethyl)-, diethyl ester<br>Diethyl 2-cyanomalonate |
| Inchi:               | InChI=1S/C10H15NO4/c1-3-14-9(12)8(6-5-7-11)10(13)15-4-2/h8H,3-6H2,1-2H3                                        |
| InchiKey:            | YJJLOESDBPRZIP-UHFFFAOYSA-N                                                                                    |
| Formula:             | C10H15NO4                                                                                                      |
| SMILES:              | CCOC(=O)C(CCC#N)C(=O)OCC                                                                                       |
| Mol. weight [g/mol]: | 213.23                                                                                                         |
| CAS:                 | 17216-62-5                                                                                                     |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -303.78 | kJ/mol  | Joback Method  |
| hf            | -579.73 | kJ/mol  | Joback Method  |
| hfus          | 25.21   | kJ/mol  | Joback Method  |
| hvap          | 66.26   | kJ/mol  | Joback Method  |
| log10ws       | -1.36   |         | Crippen Method |
| logp          | 1.033   |         | Crippen Method |
| mcvol         | 168.020 | ml/mol  | McGowan Method |
| pc            | 2261.11 | kPa     | Joback Method  |
| tb            | 682.42  | K       | Joback Method  |
| tc            | 879.91  | K       | Joback Method  |
| tf            | 396.77  | K       | Joback Method  |
| vc            | 0.663   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 443.83 | J/mol×K | 682.42          | Joback Method |
| cpg           | 455.26 | J/mol×K | 715.33          | Joback Method |
| cpg           | 466.06 | J/mol×K | 748.25          | Joback Method |
| cpg           | 476.23 | J/mol×K | 781.16          | Joback Method |
| cpg           | 485.76 | J/mol×K | 814.08          | Joback Method |
| cpg           | 494.65 | J/mol×K | 846.99          | Joback Method |

cpg

502.88

J/mol×K

879.91

Joback Method

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 388.70 | K    | 0.30           | NIST Webbook |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17216625&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17216625&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| Joback Method:  | <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>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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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