

# Dimethyl bromoterephthalate

|                      |                                                                       |
|----------------------|-----------------------------------------------------------------------|
| Other names:         | Dimethyl 2-bromoterephthalate                                         |
| Inchi:               | InChI=1S/C10H9BrO4/c1-14-9(12)6-3-4-7(8(11)5-6)10(13)15-2/h3-5H,1-2H3 |
| InchiKey:            | VUMPFOPENBVFOF-UHFFFAOYSA-N                                           |
| Formula:             | C10H9BrO4                                                             |
| SMILES:              | COC(=O)c1ccc(C(=O)OC)c(Br)c1                                          |
| Mol. weight [g/mol]: | 273.08                                                                |

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.6511  |         | Cheméo Relay (1.0) |
| hf            | -605.50 | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 25.78   | kJ/mol  | Joback Method      |
| hvap          | 83.49   | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 9.46    | eV      | Cheméo Relay (1.0) |
| log10ws       | -3.77   |         | Cheméo Relay (1.0) |
| logp          | 2.022   |         | Crippen Method     |
| mcvol         | 160.380 | ml/mol  | McGowan Method     |
| pc            | 3395.98 | kPa     | Joback Method      |
| tb            | 580.19  | K       | Cheméo Relay (1.0) |
| tc            | 788.59  | K       | Cheméo Relay (1.0) |
| tf            | 345.54  | K       | Cheméo Relay (1.0) |
| vc            | 0.582   | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 370.20    | J/mol×K | 683.58          | Joback Method |
| cpg           | 380.78    | J/mol×K | 722.13          | Joback Method |
| cpg           | 390.61    | J/mol×K | 760.69          | Joback Method |
| cpg           | 399.69    | J/mol×K | 799.24          | Joback Method |
| cpg           | 408.03    | J/mol×K | 837.79          | Joback Method |
| cpg           | 415.60    | J/mol×K | 876.35          | Joback Method |
| cpg           | 422.41    | J/mol×K | 914.90          | Joback Method |
| dvisc         | 0.0008269 | Pa×s    | 458.04          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0005740 | Pa×s | 495.63 | Joback Method |
| dvisc | 0.0004196 | Pa×s | 533.22 | Joback Method |
| dvisc | 0.0003196 | Pa×s | 570.81 | Joback Method |
| dvisc | 0.0002517 | Pa×s | 608.40 | Joback Method |
| dvisc | 0.0002039 | Pa×s | 645.99 | Joback Method |
| dvisc | 0.0001690 | Pa×s | 683.58 | Joback Method |

## Sources

|                                  |                                                                                                                                               |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b>           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>Cheméo Relay (1.0):</b>       |                                                                                                                                               |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                               |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C18643862&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18643862&amp;Units=SI</a> |
| <b>Joback Method:</b>            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| <b>McGowan Method:</b>           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>                                     |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>ie:</b>      | Ionization energy                               |
| <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>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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