

# propan-2-yl propan-2-yloxy carbonyloxy carbonate

Inchi: InChI=1S/C8H14O6/c1-5(2)11-7(9)13-14-8(10)12-6(3)4/h5-6H,1-4H3  
InchiKey: BWJUFXUULUEGMA-UHFFFAOYSA-N  
Formula: C8H14O6  
SMILES: CC(C)OC(=O)OOC(=O)OC(C)C  
Mol. weight [g/mol]: 206.19  
CAS: 105-64-6

## Physical Properties

| Property code | Value    | Unit   | Source                                                           |
|---------------|----------|--------|------------------------------------------------------------------|
| hf            | -1000.49 | kJ/mol | Cheméo Relay (1.0)                                               |
| hfus          | 20.54    | kJ/mol | Joback Method                                                    |
| hvap          | 75.38    | kJ/mol | Cheméo Relay (1.0)                                               |
| ie            | 10.10    | eV     | Cheméo Relay (1.0)                                               |
| log10ws       | -2.12    |        | Cheméo Relay (1.0)                                               |
| logp          | 2.025    |        | Crippen Method                                                   |
| mcvol         | 150.200  | ml/mol | McGowan Method                                                   |
| pc            | 2515.07  | kPa    | Joback Method                                                    |
| tb            | 461.60   | K      | Cheméo Relay (1.0)                                               |
| tc            | 605.39   | K      | Cheméo Relay (1.0)                                               |
| tf            | 283.15   | K      | Jean-Claude Bradley<br>Open Melting Point<br>Dataset (2014, CC0) |

## Correlations

| Information   | Value                                                        |
|---------------|--------------------------------------------------------------|
| Property code | cpg                                                          |
| Equation      | $Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$ |
| Y unit        | J/mol×K                                                      |
| Coeff. A      | 9.40700e+01                                                  |
| Coeff. B      | 5.39680e-01                                                  |
| Coeff. C      | -6.60000e-06                                                 |
| Coeff. D      | -1.40800e-07                                                 |
| Coeff. E      | 0.00000e+00                                                  |

| Basis                       | predicted |
|-----------------------------|-----------|
| Temperature range (K), min. | 273.00    |
| Temperature range (K), max. | 1000.00   |

| Information                 | Value                                                      |
|-----------------------------|------------------------------------------------------------|
| Property code               | dvisc                                                      |
| Equation                    | $Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$         |
| Y unit                      | Pa×s                                                       |
| Coeff. A                    | -1.30792e+01                                               |
| Coeff. B                    | 2.16298e+03                                                |
| Coeff. C                    | 0.00000e+00                                                |
| Coeff. D                    | 0.00000e+00                                                |
| Coeff. E                    | 0.00000e+00                                                |
| Basis                       | predicted                                                  |
| Comment                     | Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc. |
| Temperature range (K), min. | 283.15                                                     |
| Temperature range (K), max. | 508.62                                                     |

## Sources

|                                                             |                                                                                                                                                                                         |
|-------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:                                             | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                                                               |
| Crippen Method:                                             | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |
| Cheméo Relay (1.0):                                         |                                                                                                                                                                                         |
| Cheméo Relay (1.0, beta):                                   |                                                                                                                                                                                         |
| Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): | <a href="https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637">https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637</a> |
| Joback Method:                                              | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |
| McGowan Method:                                             | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <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       |

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