

# 2-(2-BROMOETHYL)-1,3-DIOXOLANE

|                      |                                                |
|----------------------|------------------------------------------------|
| Other names:         | 1,3-Dioxolane, 2-(2-bromoethyl)-               |
| Inchi:               | InChI=1S/C5H9BrO2/c6-2-1-5-7-3-4-8-5/h5H,1-4H2 |
| InchiKey:            | GGZQLTVZPOGLCC-UHFFFAOYSA-N                    |
| Formula:             | C5H9BrO2                                       |
| SMILES:              | BrCCC1OCCO1                                    |
| Mol. weight [g/mol]: | 181.03                                         |

## Physical Properties

| Property code | Value  | Unit   | Source             |
|---------------|--------|--------|--------------------|
| hfus          | 23.88  | kJ/mol | Joback Method      |
| logp          | 1.144  |        | Crippen Method     |
| mcvol         | 99.690 | ml/mol | McGowan Method     |
| tb            | 461.92 | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 194.26    | J/mol×K | 449.14          | Joback Method |
| cpg           | 205.89    | J/mol×K | 485.56          | Joback Method |
| cpg           | 216.81    | J/mol×K | 521.98          | Joback Method |
| cpg           | 227.06    | J/mol×K | 558.40          | Joback Method |
| cpg           | 236.66    | J/mol×K | 594.82          | Joback Method |
| cpg           | 245.64    | J/mol×K | 631.24          | Joback Method |
| cpg           | 254.03    | J/mol×K | 667.66          | Joback Method |
| dvisc         | 0.0045591 | Pa×s    | 269.95          | Joback Method |
| dvisc         | 0.0026891 | Pa×s    | 299.81          | Joback Method |
| dvisc         | 0.0017453 | Pa×s    | 329.68          | Joback Method |
| dvisc         | 0.0012171 | Pa×s    | 359.54          | Joback Method |
| dvisc         | 0.0008970 | Pa×s    | 389.41          | Joback Method |
| dvisc         | 0.0006905 | Pa×s    | 419.27          | Joback Method |
| dvisc         | 0.0005503 | Pa×s    | 449.14          | Joback Method |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 342.20 | K    | 1.00           | NIST Webbook |

## Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C18742024&Units=SI>

Joback Method: [https://en.wikipedia.org/wiki/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](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

|               |                                           |
|---------------|-------------------------------------------|
| <b>cpg:</b>   | Ideal gas heat capacity                   |
| <b>dvisc:</b> | Dynamic viscosity                         |
| <b>hfus:</b>  | Enthalpy of fusion at standard conditions |
| <b>logp:</b>  | Octanol/Water partition coefficient       |
| <b>mcvol:</b> | McGowan's characteristic volume           |
| <b>tb:</b>    | Normal Boiling Point Temperature          |
| <b>tbrp:</b>  | Boiling point at reduced pressure         |

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