

# 2-(2-(2-(2-Isobutoxy-ethoxy)-ethoxy)-ethoxy)-ethoxy-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C14H30O6/c1-14(2)13-20-12-11-19-10-9-18-8-7-17-6-5-16-4-3-15/h14-15H,3-1

QTTFKAZBPNVZRR-UHFFFAOYSA-N

C14H30O6

CC(C)COCCOCCOCCOCCOCCO

294.38

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -597.26  | kJ/mol  | Joback Method  |
| hf            | -1150.90 | kJ/mol  | Joback Method  |
| hfus          | 38.52    | kJ/mol  | Joback Method  |
| hvap          | 75.10    | kJ/mol  | Joback Method  |
| log10ws       | -0.14    |         | Crippen Method |
| logp          | 0.718    |         | Crippen Method |
| mcvol         | 243.340  | ml/mol  | McGowan Method |
| pc            | 1541.49  | kPa     | Joback Method  |
| rinpol        | 2092.00  |         | NIST Webbook   |
| rinpol        | 2092.00  |         | NIST Webbook   |
| tb            | 723.56   | K       | Joback Method  |
| tc            | 891.48   | K       | Joback Method  |
| tf            | 404.51   | K       | Joback Method  |
| vc            | 0.922    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 731.91    | J/mol×K | 723.56          | Joback Method |
| cpg           | 747.59    | J/mol×K | 751.55          | Joback Method |
| cpg           | 762.54    | J/mol×K | 779.53          | Joback Method |
| cpg           | 776.75    | J/mol×K | 807.52          | Joback Method |
| cpg           | 790.21    | J/mol×K | 835.51          | Joback Method |
| cpg           | 802.90    | J/mol×K | 863.50          | Joback Method |
| cpg           | 814.81    | J/mol×K | 891.48          | Joback Method |
| dvisc         | 0.0008552 | Pa×s    | 404.51          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002714 | Pa×s | 457.69 | Joback Method |
| dvisc | 0.0001094 | Pa×s | 510.86 | Joback Method |
| dvisc | 0.0000523 | Pa×s | 564.03 | Joback Method |
| dvisc | 0.0000284 | Pa×s | 617.21 | Joback Method |
| dvisc | 0.0000170 | Pa×s | 670.38 | Joback Method |
| dvisc | 0.0000110 | Pa×s | 723.56 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R188260&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R188260&amp;Units=SI</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>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>rinpol:</b>  | Non-polar retention indices                     |
| <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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