

# METHANE, TRICHLOROiodo-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/CCl3I/c2-1(3,4)5

SFLKZLQXODICBP-UHFFFAOYSA-N

CCl3I

ClC(Cl)(Cl)I

245.27

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.1609  |         | Cheméo Relay (1.0) |
| gf            | -17.29  | kJ/mol  | Joback Method      |
| hf            | 4.72    | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 7.93    | kJ/mol  | Joback Method      |
| hvap          | 37.40   | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 9.80    | eV      | Cheméo Relay (1.0) |
| log10ws       | -2.74   |         | Cheméo Relay (1.0) |
| logp          | 2.749   |         | Crippen Method     |
| mcvol         | 87.490  | ml/mol  | McGowan Method     |
| pc            | 4903.92 | kPa     | Joback Method      |
| tb            | 400.92  | K       | Cheméo Relay (1.0) |
| tc            | 631.70  | K       | Cheméo Relay (1.0) |
| tf            | 280.16  | K       | Cheméo Relay (1.0) |
| vc            | 0.321   | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 96.93     | J/mol×K | 424.48          | Joback Method |
| cpg           | 99.46     | J/mol×K | 466.86          | Joback Method |
| cpg           | 101.45    | J/mol×K | 509.23          | Joback Method |
| cpg           | 102.97    | J/mol×K | 551.61          | Joback Method |
| cpg           | 104.07    | J/mol×K | 593.98          | Joback Method |
| cpg           | 104.84    | J/mol×K | 636.36          | Joback Method |
| cpg           | 105.31    | J/mol×K | 678.73          | Joback Method |
| dvisc         | 0.0065312 | Pa×s    | 251.27          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0035095 | Pa×s | 280.14 | Joback Method |
| dvisc | 0.0021178 | Pa×s | 309.01 | Joback Method |
| dvisc | 0.0013932 | Pa×s | 337.88 | Joback Method |
| dvisc | 0.0009790 | Pa×s | 366.74 | Joback Method |
| dvisc | 0.0007243 | Pa×s | 395.61 | Joback Method |
| dvisc | 0.0005583 | Pa×s | 424.48 | 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>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>                         |
| <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=C594229&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C594229&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <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>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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