

# 3,9-DIVINYL-2,4,8,10-TETRAOXASPIRO[5.5]UNDE

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2,4,8,10-Tetraoxaspiro[5.5]undecane, 3,9-divinyl-Acrolein pentaerythritol bisacetal<br>Acrolein-pentaerythritol dicyclic acetal<br>Acrolein, cyclic diacetal with pentaerythritol<br>Acrolein, cyclic neopentanetetrayl acetal<br>Diallylidene pentaerythritol<br>3,9-Divinyl-2,4,8,10-tetraoxaspiro[5.5]undecane<br>3,9-Divinyl-2,4,8,10,tetraoxaspiro(5,5)undecane<br>3,9-Divinylspirobi(m-dioxane)<br>NSC 7585<br>Pentaerythritol diacrolein acetal |
| Inchi:               | InChI=1S/C11H16O4/c1-3-9-12-5-11(6-13-9)7-14-10(4-2)15-8-11/h3-4,9-10H,1-2,5-8H2                                                                                                                                                                                                                                                                                                                                                                       |
| InchiKey:            | OOXMQACSWCZQLX-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                                                                                            |
| Formula:             | C11H16O4                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| SMILES:              | C=CC1OCC2(CO1)COC(C=C)OC2                                                                                                                                                                                                                                                                                                                                                                                                                              |
| Mol. weight [g/mol]: | 212.25                                                                                                                                                                                                                                                                                                                                                                                                                                                 |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hfus          | 34.14   | kJ/mol | Joback Method  |
| logp          | 1.091   |        | Crippen Method |
| mcvol         | 159.010 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 431.61 | J/mol×K | 582.64          | Joback Method |
| cpg           | 450.90 | J/mol×K | 622.24          | Joback Method |
| cpg           | 468.84 | J/mol×K | 661.84          | Joback Method |
| cpg           | 485.58 | J/mol×K | 701.44          | Joback Method |
| cpg           | 501.30 | J/mol×K | 741.04          | Joback Method |
| cpg           | 516.16 | J/mol×K | 780.63          | Joback Method |
| cpg           | 530.31 | J/mol×K | 820.23          | Joback Method |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 382.20 | K    | 0.30           | NIST Webbook |

## Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C78193&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)

Cheméo Relay (1.0):

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/86-613-6/3-9-DIVINYL-2-4-8-10-TETRAOXASPIRO-5-5-UNDECANE.pdf>

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