

# 3,7-Guaiadiene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h6-7,10-11,14-15H,5,8-9

YOIKPWLIIDGZLM-UHFFFAOYSA-N

C15H24

CC1=CCC2C(C)CC=C(C(C)C)CC12

204.35

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | 179.03  | kJ/mol | Joback Method  |
| hf            | -164.97 | kJ/mol | Joback Method  |
| hfus          | 21.69   | kJ/mol | Joback Method  |
| hvap          | 50.71   | kJ/mol | Joback Method  |
| log10ws       | -4.63   |        | Crippen Method |
| logp          | 4.581   |        | Crippen Method |
| mcvol         | 191.890 | ml/mol | McGowan Method |
| pc            | 1921.98 | kPa    | Joback Method  |
| rinpol        | 1444.00 |        | NIST Webbook   |
| rinpol        | 1461.00 |        | NIST Webbook   |
| rinpol        | 1461.00 |        | NIST Webbook   |
| rinpol        | 1442.00 |        | NIST Webbook   |
| rinpol        | 1414.00 |        | NIST Webbook   |
| rinpol        | 1414.00 |        | NIST Webbook   |
| rinpol        | 1444.00 |        | NIST Webbook   |
| ripol         | 1810.00 |        | NIST Webbook   |
| ripol         | 1810.00 |        | NIST Webbook   |
| ripol         | 1811.00 |        | NIST Webbook   |
| ripol         | 1810.00 |        | NIST Webbook   |
| ripol         | 1811.00 |        | NIST Webbook   |
| ripol         | 1811.00 |        | NIST Webbook   |
| ripol         | 1811.00 |        | NIST Webbook   |
| ripol         | 1810.00 |        | NIST Webbook   |
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| ripol         | 1810.00 |        | NIST Webbook   |
| ripol         | 1810.00 |        | NIST Webbook   |
| ripol         | 1811.00 |        | NIST Webbook   |
| ripol         | 1810.00 |        | NIST Webbook   |
| ripol         | 1810.00 |        | NIST Webbook   |
| ripol         | 1810.00 |        | NIST Webbook   |

|       |         |                      |               |
|-------|---------|----------------------|---------------|
| ripol | 1810.00 |                      | NIST Webbook  |
| ripol | 1810.00 |                      | NIST Webbook  |
| tb    | 576.33  | K                    | Joback Method |
| tc    | 791.72  | K                    | Joback Method |
| tf    | 287.93  | K                    | Joback Method |
| vc    | 0.723   | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 503.29    | J/mol×K | 576.33          | Joback Method |
| cpg           | 604.51    | J/mol×K | 755.83          | Joback Method |
| cpg           | 586.71    | J/mol×K | 719.93          | Joback Method |
| cpg           | 567.74    | J/mol×K | 684.03          | Joback Method |
| cpg           | 547.54    | J/mol×K | 648.13          | Joback Method |
| cpg           | 526.08    | J/mol×K | 612.23          | Joback Method |
| cpg           | 621.19    | J/mol×K | 791.72          | Joback Method |
| dvisc         | 0.0003401 | Pa×s    | 576.33          | Joback Method |
| dvisc         | 0.0004008 | Pa×s    | 528.26          | Joback Method |
| dvisc         | 0.0004882 | Pa×s    | 480.20          | Joback Method |
| dvisc         | 0.0006213 | Pa×s    | 432.13          | Joback Method |
| dvisc         | 0.0008398 | Pa×s    | 384.06          | Joback Method |
| dvisc         | 0.0012375 | Pa×s    | 336.00          | Joback Method |
| dvisc         | 0.0020754 | Pa×s    | 287.93          | Joback Method |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R286196&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R286196&amp;Units=SI</a> |
| 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>                         |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

**cpg:** 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>ripol:</b>   | 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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