

# Cyclohexasilane, dodecamethyl-

|                      |                                                                             |
|----------------------|-----------------------------------------------------------------------------|
| Other names:         | Dodecamethylcyclohexasilane<br>Dodecamethylcyclohexasilylene                |
| Inchi:               | InChI=1S/C12H36Si6/c1-13(2)14(3,4)16(7,8)18(11,12)17(9,10)15(13,5)6/h1-12H3 |
| InchiKey:            | RTCLHEHPUHREBC-UHFFFAOYSA-N                                                 |
| Formula:             | C12H36Si6                                                                   |
| SMILES:              | C[Si]1(C)[Si](C)(C)[Si](C)(C)[Si](C)(C)[Si](C)(C)[Si]1(C)C                  |
| Mol. weight [g/mol]: | 348.93                                                                      |
| CAS:                 | 4098-30-0                                                                   |

## Physical Properties

| Property code | Value         | Unit | Source         |
|---------------|---------------|------|----------------|
| ie            | 7.29 ± 0.01   | eV   | NIST Webbook   |
| ie            | 7.79          | eV   | NIST Webbook   |
| log10ws       | 9.40          |      | Crippen Method |
| logp          | 4.721         |      | Crippen Method |
| rinpol        | 1593.00       |      | NIST Webbook   |
| rinpol        | 1593.00       |      | NIST Webbook   |
| tf            | 528.80 ± 0.10 | K    | NIST Webbook   |

## Temperature Dependent Properties

| Property code | Value | Unit   | Temperature [K] | Source       |
|---------------|-------|--------|-----------------|--------------|
| hfust         | 4.20  | kJ/mol | 528.80          | NIST Webbook |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| 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>                           |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4098300&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4098300&amp;Units=SI</a> |

# Legend

|                 |                                           |
|-----------------|-------------------------------------------|
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature |
| <b>ie:</b>      | Ionization energy                         |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l        |
| <b>logp:</b>    | Octanol/Water partition coefficient       |
| <b>rmpol:</b>   | Non-polar retention indices               |
| <b>tf:</b>      | Normal melting (fusion) point             |

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