

# trans-«alpha»-bergaptene

**Inchi:** InChI=1S/C15H24/c1-11(2)6-5-9-15(4)13-8-7-12(3)14(15)10-13/h6-7,13-14H,5,8-10H2,1  
**InchiKey:** YMBFCQPIMVLNIU-GRKKQISMSA-N  
**Formula:** C15H24  
**SMILES:** CC(C)=CCCC1(C)C2CC=C(C)C1C2  
**Mol. weight [g/mol]:** 204.35

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hfus          | 23.27   | kJ/mol | Joback Method      |
| hvap          | 63.46   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 7.90    | eV     | Cheméo Relay (1.0) |
| logp          | 4.725   |        | Crippen Method     |
| mcvol         | 191.890 | ml/mol | McGowan Method     |
| rinpol        | 1436.00 |        | NIST Webbook       |
| rinpol        | 1440.00 |        | NIST Webbook       |
| rinpol        | 1440.00 |        | NIST Webbook       |
| tb            | 536.39  | K      | Cheméo Relay (1.0) |
| tf            | 239.35  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 496.98 | J/mol×K | 564.10          | Joback Method |
| cpg           | 517.47 | J/mol×K | 598.66          | Joback Method |
| cpg           | 536.69 | J/mol×K | 633.23          | Joback Method |
| cpg           | 554.80 | J/mol×K | 667.79          | Joback Method |
| cpg           | 571.95 | J/mol×K | 702.35          | Joback Method |
| cpg           | 588.31 | J/mol×K | 736.92          | Joback Method |
| cpg           | 604.03 | J/mol×K | 771.48          | Joback Method |

# Sources

|                                  |                                                                                                                                           |
|----------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R239695&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R239695&amp;Units=SI</a> |
| <b>Joback Method:</b>            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

# Legend

|                |                                                 |
|----------------|-------------------------------------------------|
| <b>cpg:</b>    | Ideal gas heat capacity                         |
| <b>hfus:</b>   | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>   | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>     | Ionization energy                               |
| <b>logp:</b>   | Octanol/Water partition coefficient             |
| <b>mcvol:</b>  | McGowan's characteristic volume                 |
| <b>rinpol:</b> | Non-polar retention indices                     |
| <b>tb:</b>     | Normal Boiling Point Temperature                |
| <b>tf:</b>     | Normal melting (fusion) point                   |

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