

# Lycopene

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | (all-E)-2,6,10,14,19,23,27,31-Octamethyl-2,6,8,10,12,14,16,18,20,22,24,26,30-dotriacontatriene, .psi.,.psi.-carotene<br>2,6,8,10,12,14,16,18,20,22,24,26,30-Dotriacontatridecaene,<br>2,6,10,14,19,23,27,31-Octamethyl-<br>2,6,8,10,12,14,16,18,20,22,24,26,30-Dotriacontatridecaene,<br>2,6,10,14,19,23,27,31-Octamethyl-, (all-E)-<br>C.I. 75125<br>Lycopene 7<br>Lycopene, all-trans-<br>NSC 407322<br>all-trans-lycopene<br>psi,psi-Carotene<br>trans-lycopene<br>«psi», «psi»-Carotene |
| <b>Inchi:</b>               | InChI=1S/C40H56/c1-33(2)19-13-23-37(7)27-17-31-39(9)29-15-25-35(5)21-11-12-22-36(6)   |
| <b>InchiKey:</b>            | OAIJSZIZWZSQBC-GYZMGTAESA-N   |
| <b>Formula:</b>             | C40H56  |
| <b>SMILES:</b>              | CC(C)=CCCC(C)=CC=CC(C)=CC=CC(C)=CC=CC=C(C)C=CC=C(C)C=CC=C(C)CCC=C   |
| <b>Mol. weight [g/mol]:</b> | 536.87  |
| <b>CAS:</b>                 | 502-65-8  |

## Physical Properties

| Property code | Value   | Unit    | Source   |
|---------------|---------|---------|--|
| gf            | 1260.38 | kJ/mol  | Joback Method  |
| hf            | 576.61  | kJ/mol  | Joback Method  |
| hfus          | 91.50   | kJ/mol  | Joback Method  |
| hvap          | 104.73  | kJ/mol  | Joback Method  |
| log10ws       | -14.66  |         | Crippen Method   |
| logp          | 12.938  |         | Crippen Method   |
| mcvol         | 518.560 | ml/mol  | McGowan Method   |
| pc            | 530.42  | kPa     | Joback Method  |
| tb            | 1167.72 | K       | Joback Method  |
| tc            | 1435.92 | K       | Joback Method  |
| tf            | 450.00  | K       | Solubility of carotenoid pigments (lycopene and astaxanthin) in supercritical carbon dioxide |
| vc            | 2.023   | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1828.25 | J/mol×K | 1167.72         | Joback Method |
| cpg           | 1871.10 | J/mol×K | 1212.42         | Joback Method |
| cpg           | 1916.84 | J/mol×K | 1257.12         | Joback Method |
| cpg           | 1966.07 | J/mol×K | 1301.82         | Joback Method |
| cpg           | 2019.37 | J/mol×K | 1346.52         | Joback Method |
| cpg           | 2077.32 | J/mol×K | 1391.22         | Joback Method |
| cpg           | 2140.51 | J/mol×K | 1435.92         | 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>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C502658&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C502658&amp;Units=SI</a> |
| <b>Crippen Method:</b>   | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>Solubility of carotenoid pigments (lycopene and astaxanthin) in supercritical carbon dioxide:</b> | <a href="https://www.doi.org/10.1016/j.fluid.2006.05.031">https://www.doi.org/10.1016/j.fluid.2006.05.031</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>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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |

**vc:** Critical Volume

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