

# 16-Heptatricosene, 25-methyl

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C38H76/c1-4-6-8-10-12-14-16-17-18-19-20-21-22-23-24-25-26-27-29-31-33-35 |
| <b>InchiKey:</b>            | UGCYHMKWCKGTR-OCOZRVBESA-N  |
| <b>Formula:</b>             | C38H76  |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCC=CCCCCCCC(C)CCCCCCCCCCCC  |
| <b>Mol. weight [g/mol]:</b> | 533.01  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 346.86  | kJ/mol               | Joback Method  |
| hf            | -715.71 | kJ/mol               | Joback Method  |
| hfus          | 90.86   | kJ/mol               | Joback Method  |
| hvap          | 99.75   | kJ/mol               | Joback Method  |
| log10ws       | -15.34  |                      | Crippen Method |
| logp          | 14.702  |                      | Crippen Method |
| mvol          | 541.980 | ml/mol               | McGowan Method |
| pc            | 432.94  | kPa                  | Joback Method  |
| rinpol        | 3696.00 |                      | NIST Webbook   |
| rinpol        | 3696.00 |                      | NIST Webbook   |
| tb            | 1072.56 | K                    | Joback Method  |
| tc            | 1385.66 | K                    | Joback Method  |
| tf            | 497.94  | K                    | Joback Method  |
| vc            | 2.138   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 2007.56   | J/molxK | 1072.56         | Joback Method |
| cpg           | 2045.43   | J/molxK | 1124.74         | Joback Method |
| cpg           | 2080.66   | J/molxK | 1176.93         | Joback Method |
| cpg           | 2113.68   | J/molxK | 1229.11         | Joback Method |
| cpg           | 2144.88   | J/molxK | 1281.30         | Joback Method |
| cpg           | 2174.70   | J/molxK | 1333.48         | Joback Method |
| cpg           | 2203.55   | J/molxK | 1385.66         | Joback Method |
| dvisc         | 0.0003678 | Paxs    | 497.94          | Joback Method |

|       |           |      |         |               |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0001039 | Paxs | 593.71  | Joback Method |
| dvisc | 0.0000417 | Paxs | 689.48  | Joback Method |
| dvisc | 0.0000209 | Paxs | 785.25  | Joback Method |
| dvisc | 0.0000122 | Paxs | 881.02  | Joback Method |
| dvisc | 0.0000079 | Paxs | 976.79  | Joback Method |
| dvisc | 0.0000055 | Paxs | 1072.56 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R608556&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R608556&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>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | 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>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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