

# trans-Cinnamamide, N,N-diheptyl-3-trifluoromethyl-

Inchi: InChI=1S/C24H36F3NO/c1-3-5-7-9-11-18-28(19-12-10-8-6-4-2)23(29)17-16-21-14-13-15

InchiKey: DUFNHAHLLWVCAY-WUKNDPDISA-N

Formula: C24H36F3NO

SMILES: CCCCCCN(CCCCCC)C(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 411.54

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -265.53 | kJ/mol  | Joback Method  |
| hf            | -838.54 | kJ/mol  | Joback Method  |
| hfus          | 58.22   | kJ/mol  | Joback Method  |
| hvap          | 76.96   | kJ/mol  | Joback Method  |
| log10ws       | -8.02   |         | Crippen Method |
| logp          | 7.488   |         | Crippen Method |
| mcvol         | 337.820 | ml/mol  | McGowan Method |
| pc            | 971.09  | kPa     | Joback Method  |
| rinpol        | 2634.00 |         | NIST Webbook   |
| tb            | 845.23  | K       | Joback Method  |
| tc            | 1037.42 | K       | Joback Method  |
| tf            | 480.69  | K       | Joback Method  |
| vc            | 1.319   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1075.75 | J/mol×K | 845.23          | Joback Method |
| cpg           | 1093.94 | J/mol×K | 877.26          | Joback Method |
| cpg           | 1111.12 | J/mol×K | 909.29          | Joback Method |
| cpg           | 1127.38 | J/mol×K | 941.32          | Joback Method |
| cpg           | 1142.82 | J/mol×K | 973.35          | Joback Method |
| cpg           | 1157.51 | J/mol×K | 1005.39         | Joback Method |
| cpg           | 1171.56 | J/mol×K | 1037.42         | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U308074&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308074&amp;Units=SI</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>hvac:</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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