

Tetracosyl pentafluoropropionate

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|-----------------------------|---|
| Other names: | Tetracosyl 2,2,3,3,3-pentafluoropropanoate 1-Tetracosanol, pentafluoropropionate |
| Inchi: | InChI=1S/C27H49F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23 |
| InchiKey: | KOPXDFYIILHNCR-UHFFFAOYSA-N |
| Formula: | C27H49F5O2 |
| SMILES: | CCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F |
| Mol. weight [g/mol]: | 500.67 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| gf | -1025.83 | kJ/mol | Joback Method |
| hf | -1843.46 | kJ/mol | Joback Method |
| hfus | 69.05 | kJ/mol | Joback Method |
| hvap | 78.17 | kJ/mol | Joback Method |
| log10ws | -10.96 | | Crippen Method |
| logp | 10.329 | | Crippen Method |
| mcvol | 407.580 | ml/mol | McGowan Method |
| pc | 640.60 | kPa | Joback Method |
| rinpol | 2580.30 | | NIST Webbook |
| rinpol | 2580.30 | | NIST Webbook |
| tb | 883.34 | K | Joback Method |
| tc | 1092.29 | K | Joback Method |
| tf | 474.00 | K | Joback Method |
| vc | 1.639 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1385.41 | J/molxK | 883.34 | Joback Method |
| cpg | 1408.73 | J/molxK | 918.16 | Joback Method |
| cpg | 1430.62 | J/molxK | 952.99 | Joback Method |
| cpg | 1451.19 | J/molxK | 987.81 | Joback Method |
| cpg | 1470.54 | J/molxK | 1022.64 | Joback Method |
| cpg | 1488.78 | J/molxK | 1057.46 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U351813&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/27-193-8/Tetracosyl-pentafluoropropionate.pdf>

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