

# «beta»-Alanine, n-heptafluorobutyryl-, hexadecyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C23H38F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-34-19(32)16-17-31-2

KYDONHMBRSQUMJ-UHFFFAOYSA-N

C23H38F7NO3

CCCCCCCCCCCCCCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)C(F)(F)F

509.54

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -1485.82 | kJ/mol  | Joback Method  |
| hf            | -2220.98 | kJ/mol  | Joback Method  |
| hfus          | 64.13    | kJ/mol  | Joback Method  |
| hvap          | 79.52    | kJ/mol  | Joback Method  |
| log10ws       | -8.57    |         | Crippen Method |
| logp          | 7.350    |         | Crippen Method |
| mcvol         | 366.310  | ml/mol  | McGowan Method |
| pc            | 788.16   | kPa     | Joback Method  |
| rinpol        | 2462.00  |         | NIST Webbook   |
| rinpol        | 2462.00  |         | NIST Webbook   |
| tb            | 891.17   | K       | Joback Method  |
| tc            | 1098.21  | K       | Joback Method  |
| tf            | 535.11   | K       | Joback Method  |
| vc            | 1.482    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1238.46 | J/mol×K | 891.17          | Joback Method |
| cpg           | 1257.05 | J/mol×K | 925.68          | Joback Method |
| cpg           | 1274.47 | J/mol×K | 960.18          | Joback Method |
| cpg           | 1290.82 | J/mol×K | 994.69          | Joback Method |
| cpg           | 1306.22 | J/mol×K | 1029.19         | Joback Method |
| cpg           | 1320.77 | J/mol×K | 1063.70         | Joback Method |
| cpg           | 1334.60 | J/mol×K | 1098.21         | 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=U320987&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320987&amp;Units=SI</a> |
| <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>                                     |

# 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>rinpola:</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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