

L-Valine, N-(3-bromobenzoyl)-, decyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C22H34BrNO3/c1-4-5-6-7-8-9-10-11-15-27-22(26)20(17(2)3)24-21(25)18-13-1 |
| InchiKey: | DRPWVWMEBOPNPV-UHFFFAOYSA-N |
| Formula: | C22H34BrNO3 |
| SMILES: | CCCCCCCCCOC(=O)C(NC(=O)c1cccc(Br)c1)C(C)C |
| Mol. weight [g/mol]: | 440.41 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -26.87 | kJ/mol | Joback Method |
| hf | -560.49 | kJ/mol | Joback Method |
| hfus | 54.11 | kJ/mol | Joback Method |
| hvap | 95.50 | kJ/mol | Joback Method |
| log10ws | -7.57 | | Crippen Method |
| logp | 5.887 | | Crippen Method |
| mcvol | 333.570 | ml/mol | McGowan Method |
| pc | 1269.16 | kPa | Joback Method |
| rinpol | 2954.00 | | NIST Webbook |
| rinpol | 2954.00 | | NIST Webbook |
| tb | 980.03 | K | Joback Method |
| tc | 1202.22 | K | Joback Method |
| tf | 581.19 | K | Joback Method |
| vc | 1.274 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1068.21 | J/mol×K | 980.03 | Joback Method |
| cpg | 1083.00 | J/mol×K | 1017.06 | Joback Method |
| cpg | 1096.58 | J/mol×K | 1054.09 | Joback Method |
| cpg | 1109.03 | J/mol×K | 1091.13 | Joback Method |
| cpg | 1120.42 | J/mol×K | 1128.16 | Joback Method |
| cpg | 1130.81 | J/mol×K | 1165.19 | Joback Method |
| cpg | 1140.26 | J/mol×K | 1202.22 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U346692&Units=SI |
| 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 |

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 |
| hvp: | 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 |
| rinp: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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