

Terephthalic acid, isobutyl 3-nitro-4-methylbenzyl ester

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| Inchi: | InChI=1S/C20H21NO6/c1-13(2)11-26-19(22)16-6-8-17(9-7-16)20(23)27-12-15-5-4-14(3) |
| InchiKey: | GFVZXQNTIICXOE-UHFFFAOYSA-N |
| Formula: | C20H21NO6 |
| SMILES: | <chem>Cc1ccc(COC(=O)c2ccc(C(=O)OCC(C)C)cc2)cc1[N+](=O)[O-]</chem> |
| Mol. weight [g/mol]: | 371.38 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -121.28 | kJ/mol | Joback Method |
| hf | -523.12 | kJ/mol | Joback Method |
| hfus | 47.88 | kJ/mol | Joback Method |
| hvap | 101.17 | kJ/mol | Joback Method |
| log10ws | -6.21 | | Crippen Method |
| logp | 4.073 | | Crippen Method |
| mvol | 277.440 | ml/mol | McGowan Method |
| pc | 1723.16 | kPa | Joback Method |
| rinpol | 3076.00 | | NIST Webbook |
| rinpol | 3076.00 | | NIST Webbook |
| tb | 1029.28 | K | Joback Method |
| tc | 1276.97 | K | Joback Method |
| tf | 678.49 | K | Joback Method |
| vc | 1.063 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 874.56 | J/mol×K | 1029.28 | Joback Method |
| cpg | 884.21 | J/mol×K | 1070.56 | Joback Method |
| cpg | 892.35 | J/mol×K | 1111.84 | Joback Method |
| cpg | 899.01 | J/mol×K | 1153.13 | Joback Method |
| cpg | 904.24 | J/mol×K | 1194.41 | Joback Method |
| cpg | 908.08 | J/mol×K | 1235.69 | Joback Method |
| cpg | 910.57 | J/mol×K | 1276.97 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U416087&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.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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