

Terephthalic acid, 4-bromobenzyl butyl ester

Inchi: InChI=1S/C19H19BrO4/c1-2-3-12-23-18(21)15-6-8-16(9-7-15)19(22)24-13-14-4-10-17(20)
InchiKey: ZTJWGIAOOMSSDP-UHFFFAOYSA-N
Formula: C19H19BrO4
SMILES: CCCOC(=O)c1ccc(C(=O)OCc2ccc(Br)cc2)cc1
Mol. weight [g/mol]: 391.26

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -138.86 | kJ/mol | Joback Method |
| hf | -448.64 | kJ/mol | Joback Method |
| hfus | 43.13 | kJ/mol | Joback Method |
| hvap | 88.51 | kJ/mol | Joback Method |
| log10ws | -6.49 | | Crippen Method |
| logp | 4.763 | | Crippen Method |
| mvol | 263.430 | ml/mol | McGowan Method |
| pc | 1977.07 | kPa | Joback Method |
| rinpol | 2970.00 | | NIST Webbook |
| rinpol | 2970.00 | | NIST Webbook |
| tb | 916.18 | K | Joback Method |
| tc | 1152.18 | K | Joback Method |
| tf | 585.89 | K | Joback Method |
| vc | 0.994 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 756.39 | J/molxK | 916.18 | Joback Method |
| cpg | 804.63 | J/molxK | 1112.85 | Joback Method |
| cpg | 797.27 | J/molxK | 1073.52 | Joback Method |
| cpg | 788.81 | J/molxK | 1034.18 | Joback Method |
| cpg | 779.21 | J/molxK | 994.85 | Joback Method |
| cpg | 768.42 | J/molxK | 955.51 | Joback Method |
| cpg | 810.93 | J/molxK | 1152.18 | Joback Method |
| dvisc | 0.0000523 | Paxs | 916.18 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000649 | Paxs | 861.13 | Joback Method |
| dvisc | 0.0000829 | Paxs | 806.08 | Joback Method |
| dvisc | 0.0001097 | Paxs | 751.03 | Joback Method |
| dvisc | 0.0001518 | Paxs | 695.99 | Joback Method |
| dvisc | 0.0002222 | Paxs | 640.94 | Joback Method |
| dvisc | 0.0003492 | Paxs | 585.89 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U415960&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| 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/99-687-1/Terephthalic-acid-4-bromobenzyl-butyl-ester.pdf>

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