

2,4,6-tribromo-3-methylphenyl trifluoroacetate

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| Other names: | 2,4,6-Tribromo-3-trifluoroacetyloxytoluene 2,4,6-Tribromo-m-cresol trifluoroacetate |
| Inchi: | InChI=1S/C9H4Br3F3O2/c1-3-4(10)2-5(11)7(6(3)12)17-8(16)9(13,14)15/h2H,1H3 |
| InchiKey: | AOOXTTARAUMVQT-UHFFFAOYSA-N |
| Formula: | C9H4Br3F3O2 |
| SMILES: | Cc1c(Br)cc(Br)c(OC(=O)C(F)(F)F)c1Br |
| Mol. weight [g/mol]: | 440.83 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -673.76 | kJ/mol | Joback Method |
| hf | -801.33 | kJ/mol | Joback Method |
| hfus | 32.02 | kJ/mol | Joback Method |
| hvap | 65.27 | kJ/mol | Joback Method |
| log10ws | -6.41 | | Crippen Method |
| logp | 4.750 | | Crippen Method |
| mcvol | 179.160 | ml/mol | McGowan Method |
| pc | 3568.53 | kPa | Joback Method |
| rinpol | 1660.00 | | NIST Webbook |
| tb | 721.27 | K | Joback Method |
| tc | 958.77 | K | Joback Method |
| tf | 523.44 | K | Joback Method |
| vc | 0.684 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 371.16 | J/molxK | 721.27 | Joback Method |
| cpg | 378.29 | J/molxK | 760.85 | Joback Method |
| cpg | 384.80 | J/molxK | 800.44 | Joback Method |
| cpg | 390.77 | J/molxK | 840.02 | Joback Method |
| cpg | 396.23 | J/molxK | 879.60 | Joback Method |
| cpg | 401.26 | J/molxK | 919.18 | Joback Method |
| cpg | 405.89 | J/molxK | 958.77 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U373437&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |

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

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