

1-Bromo-2,4,6-trichlorobenzene

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|-----------------------------|--|
| Inchi: | InChI=1S/C6H2BrCl3/c7-6-4(9)1-3(8)2-5(6)10/h1-2H |
| InchiKey: | BAPPAFMEUDJAQI-UHFFFAOYSA-N |
| Formula: | C6H2BrCl3 |
| SMILES: | Clc1cc(Cl)c(Br)c(Cl)c1 |
| Mol. weight [g/mol]: | 260.34 |
| CAS: | 19393-96-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 61.69 | kJ/mol | Joback Method |
| hf | 14.06 | kJ/mol | Joback Method |
| hfus | 22.05 | kJ/mol | Joback Method |
| hvap | 52.80 | kJ/mol | Joback Method |
| log10ws | -4.69 | | Crippen Method |
| logp | 4.409 | | Crippen Method |
| mcvol | 125.860 | ml/mol | McGowan Method |
| pc | 4162.33 | kPa | Joback Method |
| tb | 556.75 | K | Joback Method |
| tc | 813.68 | K | Joback Method |
| tf | 370.92 | K | Joback Method |
| vc | 0.472 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 192.28 | J/molxK | 556.75 | Joback Method |
| cpg | 198.31 | J/molxK | 599.57 | Joback Method |
| cpg | 203.83 | J/molxK | 642.39 | Joback Method |
| cpg | 208.89 | J/molxK | 685.21 | Joback Method |
| cpg | 213.52 | J/molxK | 728.04 | Joback Method |
| cpg | 217.75 | J/molxK | 770.86 | Joback Method |
| cpg | 221.63 | J/molxK | 813.68 | Joback Method |
| dvisc | 0.0012470 | Paxs | 370.92 | Joback Method |
| dvisc | 0.0009030 | Paxs | 401.89 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0006848 | Paxs | 432.86 | Joback Method |
| dvisc | 0.0005388 | Paxs | 463.84 | Joback Method |
| dvisc | 0.0004369 | Paxs | 494.81 | Joback Method |
| dvisc | 0.0003631 | Paxs | 525.78 | Joback Method |
| dvisc | 0.0003081 | Paxs | 556.75 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C19393965&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 |

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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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