

1,2,6-tribromo,3-chloro-dibenzo-dioxin

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|-----------------------------|---|
| Inchi: | InChI=1S/C12H4Br3ClO2/c13-5-2-1-3-7-11(5)18-8-4-6(16)9(14)10(15)12(8)17-7/h1-4H |
| InchiKey: | DEHHOFOEWLXSSV-UHFFFAOYSA-N |
| Formula: | C12H4Br3ClO2 |
| SMILES: | Clc1cc2c(c(Br)c1Br)Oc1cccc(Br)c1O2 |
| Mol. weight [g/mol]: | 455.32 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 156.55 | kJ/mol | Joback Method |
| hf | 11.78 | kJ/mol | Joback Method |
| hfus | 47.76 | kJ/mol | Joback Method |
| hvap | 83.59 | kJ/mol | Joback Method |
| log10ws | -7.16 | | Crippen Method |
| logp | 6.526 | | Crippen Method |
| mcvol | 198.040 | ml/mol | McGowan Method |
| pc | 4397.41 | kPa | Joback Method |
| rinpol | 2705.00 | | NIST Webbook |
| tb | 854.15 | K | Joback Method |
| tc | 1144.33 | K | Joback Method |
| tf | 641.12 | K | Joback Method |
| vc | 0.735 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 407.09 | J/molxK | 854.15 | Joback Method |
| cpg | 414.50 | J/molxK | 902.51 | Joback Method |
| cpg | 421.68 | J/molxK | 950.88 | Joback Method |
| cpg | 428.84 | J/molxK | 999.24 | Joback Method |
| cpg | 436.15 | J/molxK | 1047.60 | Joback Method |
| cpg | 443.83 | J/molxK | 1095.96 | Joback Method |
| cpg | 452.05 | J/molxK | 1144.33 | Joback Method |
| dvisc | 0.0009125 | Paxs | 641.12 | Joback Method |
| dvisc | 0.0007623 | Paxs | 676.62 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0006483 | Paxs | 712.13 | Joback Method |
| dvisc | 0.0005599 | Paxs | 747.63 | Joback Method |
| dvisc | 0.0004901 | Paxs | 783.14 | Joback Method |
| dvisc | 0.0004339 | Paxs | 818.64 | Joback Method |
| dvisc | 0.0003881 | Paxs | 854.15 | 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=R172399&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 |

Latest version available from:

<https://www.chemeo.com/cid/34-298-4/1-2-6-tribromo-3-chloro-dibenzo-dioxin.pdf>

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