# 3,4-DICHLOROBENZOTRIFLUORIDE

**Other names:** 3,4-dichloro-«alpha»,«alpha»,«alpha»-trifluorotoluene
Benzene, 1,2-dichloro-4-(trifluoromethyl)-
**Inchi:** InChI=1S/C7H3Cl2F3/c8-5-2-1-4(3-6(5)9)7(10,11)12/h1-3H
**InchiKey:** XILPLWOGHPSJBK-UHFFFAOYSA-N
**Formula:** C7H3Cl2F3
**SMILES:** FC(F)(F)c1ccc(Cl)c(Cl)c1
**Mol. weight [g/mol]:** 215.00
**CAS:** 328-84-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -640.44 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 17.37 | kJ/mol | Joback Method |
| hvap | 51.77 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.69 | eV | Cheméo Relay (1.0) |
| log10ws | -3.69 | | Cheméo Relay (1.0) |
| logp | 4.012 | | Crippen Method |
| mcvol | 115.520 | ml/mol | McGowan Method |
| tb | 446.70 | K | NIST Webbook |
| tb | 446.50 ± 0.50 | K | NIST Webbook |
| tf | 300.73 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 215.20 | J/mol×K | 465.64 | Joback Method |
| cpg | 224.05 | J/mol×K | 500.26 | Joback Method |
| cpg | 232.21 | J/mol×K | 534.89 | Joback Method |
| cpg | 239.74 | J/mol×K | 569.51 | Joback Method |
| cpg | 246.66 | J/mol×K | 604.14 | Joback Method |
| cpg | 253.01 | J/mol×K | 638.76 | Joback Method |
| cpg | 258.84 | J/mol×K | 673.39 | Joback Method |
| hvapt | 44.10 | kJ/mol | 403.00 | NIST Webbook |
| hvapt | 41.80 | kJ/mol | 365.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.74419e+01 |
| Coeff. B | -6.07136e+03 |
| Coeff. C | 2.68530e+01 |
| Temperature range (K), min. | 327.07 |
| Temperature range (K), max. | 473.65 |

# Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C328847&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pvap:** | Vapor pressure |

**tb:** Normal Boiling Point Temperature

**tf:** Normal melting (fusion) point