# Benzaldehyde, 3-(trifluoromethyl)-

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|---|---|
| **Other names:** | 3-Trifluoromethylbenzaldehyde<br>m-Trifluoromethylbenzaldehyde<br>«alpha» «alpha» «alpha»-Trifluoro-m-tolualdehyde<br>m-Tolualdehyde, «alpha»,«alpha»,«alpha»-trifluoro-<br>«alpha»,«alpha»,«alpha»-trifluoro-3-tolualdehyde |
| **Inchi:** | InChI=1S/C8H5F3O/c9-8(10,11)7-3-1-2-6(4-7)5-12/h1-5H |
| **InchiKey:** | NMTUHPSKJJYGML-UHFFFAOYSA-N |
| **Formula:** | C8H5F3O |
| **SMILES:** | O=Cc1cccc(C(F)(F)F)c1 |
| **Mol. weight [g/mol]:** | 174.12 |
| **CAS:** | 454-89-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ea | 0.83 ± 0.09 | eV | NIST Webbook |
| ea | 0.81 ± 0.09 | eV | NIST Webbook |
| gf | -561.85 | kJ/mol | Joback Method |
| hf | -666.05 | kJ/mol | Joback Method |
| hfus | 14.24 | kJ/mol | Joback Method |
| hvap | 39.31 | kJ/mol | Joback Method |
| log10ws | -2.82 | | Crippen Method |
| logp | 2.518 | | Crippen Method |
| mcvol | 106.700 | ml/mol | McGowan Method |
| pc | 3411.87 | kPa | Joback Method |
| tb | 457.34 | K | Joback Method |
| tc | 654.26 | K | Joback Method |
| tf | 265.05 | K | Joback Method |
| vc | 0.435 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 222.36 | J/mol×K | 457.34 | Joback Method |
| cpg | 232.79 | J/mol×K | 490.16 | Joback Method |

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|---|---|---|---|---|
| cpg | 242.49 | J/mol×K | 522.98 | Joback Method |
| cpg | 251.50 | J/mol×K | 555.80 | Joback Method |
| cpg | 259.86 | J/mol×K | 588.62 | Joback Method |
| cpg | 267.59 | J/mol×K | 621.44 | Joback Method |
| cpg | 274.75 | J/mol×K | 654.26 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 357.70 | K | 4.00 | NIST Webbook |
| tbrp | 357.50 ± 1.50 | K | 4.00 | NIST Webbook |

# 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=C454897&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
**ea:** Electron affinity
**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
**tb:** Normal Boiling Point Temperature
**tbrp:** Boiling point at reduced pressure
**tc:** Critical Temperature

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

**vc:** Critical Volume