# 1-[(3-Trifluoromethyl)phenyl]propanol-1

**Inchi:** InChI=1S/C10H11F3O/c1-2-9(14)7-4-3-5-8(6-7)10(11,12)13/h3-6,9,14H,2H2,1H3
**InchiKey:** SZSJCUKIEPGUMF-UHFFFAOYSA-N
**Formula:** C10H11F3O
**SMILES:** CCC(O)c1cccc(C(F)(F)F)c1
**Mol. weight [g/mol]:** 204.19
**CAS:** 618-97-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -584.75 | kJ/mol | Joback Method |
| hf | -779.26 | kJ/mol | Joback Method |
| hfus | 17.70 | kJ/mol | Joback Method |
| hvap | 53.34 | kJ/mol | Joback Method |
| log10ws | -3.52 | | Crippen Method |
| logp | 3.149 | | Crippen Method |
| mcvol | 139.180 | ml/mol | McGowan Method |
| pc | 2835.36 | kPa | Joback Method |
| tb | 546.18 | K | Joback Method |
| tc | 727.80 | K | Joback Method |
| tf | 291.41 | K | Joback Method |
| vc | 0.543 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 339.99 | J/mol×K | 546.18 | Joback Method |
| cpg | 351.56 | J/mol×K | 576.45 | Joback Method |
| cpg | 362.42 | J/mol×K | 606.72 | Joback Method |
| cpg | 372.62 | J/mol×K | 636.99 | Joback Method |
| cpg | 382.19 | J/mol×K | 667.26 | Joback Method |
| cpg | 391.16 | J/mol×K | 697.53 | Joback Method |
| cpg | 399.57 | J/mol×K | 727.80 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 362.50 ± 1.50 | K | 0.70 | NIST Webbook |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C618973&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |