# Benzeneacetic acid, 3,5-bis(trifluoromethyl)-

**Other names:** 3,5-bis(trifluoromethyl)phenylacetic acid
**Inchi:** InChI=1S/C10H6F6O2/c11-9(12,13)6-1-5(3-8(17)18)2-7(4-6)10(14,15)16/h1-2,4H,3H2,(H
**InchiKey:** PAWSKKHEEYTXSA-UHFFFAOYSA-N
**Formula:** C10H6F6O2
**SMILES:** O=C(O)Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1
**Mol. weight [g/mol]:** 272.14
**CAS:** 85068-33-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1302.45 | kJ/mol | Joback Method |
| hf | -1495.11 | kJ/mol | Joback Method |
| hfus | 24.26 | kJ/mol | Joback Method |
| hvap | 57.39 | kJ/mol | Joback Method |
| log10ws | -3.58 | | Crippen Method |
| logp | 3.351 | | Crippen Method |
| mcvol | 146.060 | ml/mol | McGowan Method |
| pc | 2619.09 | kPa | Joback Method |
| tb | 600.05 | K | Joback Method |
| tc | 774.07 | K | Joback Method |
| tf | 373.05 | K | Joback Method |
| vc | 0.599 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 382.29 | J/mol×K | 600.05 | Joback Method |
| cpg | 391.29 | J/mol×K | 629.05 | Joback Method |
| cpg | 399.65 | J/mol×K | 658.06 | Joback Method |
| cpg | 407.42 | J/mol×K | 687.06 | Joback Method |
| cpg | 414.63 | J/mol×K | 716.06 | Joback Method |
| cpg | 421.32 | J/mol×K | 745.07 | Joback Method |
| cpg | 427.52 | J/mol×K | 774.07 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C85068333&Units=SI |

# Legend

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|---|---|
| **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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |