# Ethanone, 2,2,2-trifluoro-1-(2,4,6-trimethylphenyl)-

**Other names:** 2,2,2-Trifluoro-2',4',6'-trimethylacetophenone
2,2,2-Trifluoro-1-(2,4,6-trimethyl-phenyl)-ethanone
«alpha»,«alpha»,«alpha»-Trifluoro-2,4,6-trimethylacetophenone
**Inchi:** InChI=1S/C11H11F3O/c1-6-4-7(2)9(8(3)5-6)10(15)11(12,13)14/h4-5H,1-3H3
**InchiKey:** VINRTVDNUHIWCB-UHFFFAOYSA-N
**Formula:** C11H11F3O
**SMILES:** Cc1cc(C)c(C(=O)C(F)(F)F)c(C)c1
**Mol. weight [g/mol]:** 216.20
**CAS:** 313-56-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -585.25 | kJ/mol | Joback Method |
| hf | -777.91 | kJ/mol | Joback Method |
| hfus | 20.55 | kJ/mol | Joback Method |
| hvap | 47.34 | kJ/mol | Joback Method |
| log10ws | -4.22 | | Crippen Method |
| logp | 3.357 | | Crippen Method |
| mcvol | 148.970 | ml/mol | McGowan Method |
| pc | 2400.57 | kPa | Joback Method |
| tb | 541.15 | K | Joback Method |
| tc | 737.75 | K | Joback Method |
| tf | 331.83 | K | Joback Method |
| vc | 0.593 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 349.47 | J/mol×K | 541.15 | Joback Method |
| cpg | 362.18 | J/mol×K | 573.92 | Joback Method |
| cpg | 374.14 | J/mol×K | 606.68 | Joback Method |
| cpg | 385.38 | J/mol×K | 639.45 | Joback Method |
| cpg | 395.94 | J/mol×K | 672.22 | Joback Method |
| cpg | 405.85 | J/mol×K | 704.98 | Joback Method |

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|---|---|---|---|---|
| cpg | 415.14 | J/mol×K | 737.75 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C313564&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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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