# 2-(N-Ethyl-N-tolylamino)ethanol, heptafluorobutyrate

**Inchi:** InChI=1S/C15H16F7NO2/c1-3-23(11-6-4-5-10(2)9-11)7-8-25-12(24)13(16,17)14(18,19)1

**InchiKey:** PTGIOONROYONRR-UHFFFAOYSA-N

**Formula:** C15H16F7NO2

**SMILES:** CCN(CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1cccc(C)c1

**Mol. weight [g/mol]:** 375.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1300.09 | kJ/mol | Joback Method |
| hf | -1704.16 | kJ/mol | Joback Method |
| hfus | 33.38 | kJ/mol | Joback Method |
| hvap | 53.51 | kJ/mol | Joback Method |
| log10ws | -4.52 | | Crippen Method |
| logp | 4.197 | | Crippen Method |
| mcvol | 228.260 | ml/mol | McGowan Method |
| pc | 1530.66 | kPa | Joback Method |
| rinpol | 1518.00 | | NIST Webbook |
| tb | 648.19 | K | Joback Method |
| tc | 821.52 | K | Joback Method |
| tf | 413.77 | K | Joback Method |
| vc | 0.902 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 649.41 | J/mol×K | 648.19 | Joback Method |
| cpg | 663.58 | J/mol×K | 677.08 | Joback Method |
| cpg | 676.80 | J/mol×K | 705.97 | Joback Method |
| cpg | 689.14 | J/mol×K | 734.85 | Joback Method |
| cpg | 700.66 | J/mol×K | 763.74 | Joback Method |
| cpg | 711.40 | J/mol×K | 792.63 | Joback Method |
| cpg | 721.43 | J/mol×K | 821.52 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U374921&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 |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |