# Etafenone

| | |
|---|---|
| **Other names:** | 1-Propanone, 1-[2-[2-(diethylamino)ethoxy]phenyl]-3-phenyl-<br>2'-[2-(Diethylamino)ethoxy]-3-phenylpropiophenone<br>LG-11457 |
| **Inchi:** | InChI=1S/C21H27NO2/c1-3-22(4-2)16-17-24-21-13-9-8-12-19(21)20(23)15-14-18-10-6-5 |
| **InchiKey:** | OEGDFSLNGABBKJ-UHFFFAOYSA-N |
| **Formula:** | C21H27NO2 |
| **SMILES:** | CCN(CC)CCOc1ccccc1C(=O)CCc1ccccc1 |
| **Mol. weight [g/mol]:** | 325.44 |
| **CAS:** | 90-54-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 217.99 | kJ/mol | Joback Method |
| hf | -192.45 | kJ/mol | Joback Method |
| hfus | 43.65 | kJ/mol | Joback Method |
| hvap | 78.75 | kJ/mol | Joback Method |
| log10ws | -4.95 | | Crippen Method |
| logp | 4.223 | | Crippen Method |
| mcvol | 276.650 | ml/mol | McGowan Method |
| pc | 1546.35 | kPa | Joback Method |
| rinpol | 2434.00 | | NIST Webbook |
| rinpol | 2434.00 | | NIST Webbook |
| tb | 826.95 | K | Joback Method |
| tc | 1042.09 | K | Joback Method |
| tf | 496.42 | K | Joback Method |
| vc | 1.038 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 837.45 | J/mol×K | 826.95 | Joback Method |
| cpg | 854.35 | J/mol×K | 862.81 | Joback Method |
| cpg | 870.02 | J/mol×K | 898.66 | Joback Method |
| cpg | 884.52 | J/mol×K | 934.52 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 897.91 | J/mol×K | 970.38 | Joback Method |
| cpg | 910.27 | J/mol×K | 1006.23 | Joback Method |
| cpg | 921.66 | J/mol×K | 1042.09 | 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=C90540&Units=SI |

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