# MEXILETINE, M(DESAMINO-OXO-HO-)ISOMER 2, AC

**Inchi:** InChI=1S/C13H16O4/c1-8-5-12(17-11(4)15)6-9(2)13(8)16-7-10(3)14/h5-6H,7H2,1-4H3
**InchiKey:** KEZJMWTUAZTVQH-UHFFFAOYSA-N
**Formula:** C13H16O4
**SMILES:** CC(=O)COc1c(C)cc(OC(C)=O)cc1C
**Mol. weight [g/mol]:** 236.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -325.74 | kJ/mol | Joback Method |
| hf | -599.13 | kJ/mol | Joback Method |
| hfus | 27.87 | kJ/mol | Joback Method |
| hvap | 67.11 | kJ/mol | Joback Method |
| log10ws | -2.97 | | Crippen Method |
| logp | 2.197 | | Crippen Method |
| mcvol | 185.150 | ml/mol | McGowan Method |
| pc | 2293.71 | kPa | Joback Method |
| rinpol | 1735.00 | | NIST Webbook |
| rinpol | 1735.00 | | NIST Webbook |
| tb | 691.04 | K | Joback Method |
| tc | 901.40 | K | Joback Method |
| tf | 444.57 | K | Joback Method |
| vc | 0.704 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 485.63 | J/mol×K | 691.04 | Joback Method |
| cpg | 545.65 | J/mol×K | 866.34 | Joback Method |
| cpg | 535.29 | J/mol×K | 831.28 | Joback Method |
| cpg | 524.10 | J/mol×K | 796.22 | Joback Method |
| cpg | 512.08 | J/mol×K | 761.16 | Joback Method |
| cpg | 499.26 | J/mol×K | 726.10 | Joback Method |
| cpg | 555.18 | J/mol×K | 901.40 | Joback Method |
| dvisc | 0.0001327 | Pa×s | 691.04 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001615 | Pa×s | 649.96 | Joback Method |
| dvisc | 0.0002019 | Pa×s | 608.88 | Joback Method |
| dvisc | 0.0002607 | Pa×s | 567.81 | Joback Method |
| dvisc | 0.0003503 | Pa×s | 526.73 | Joback Method |
| dvisc | 0.0004947 | Pa×s | 485.65 | Joback Method |
| dvisc | 0.0007449 | Pa×s | 444.57 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R255266&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 |
| **dvisc:** | Dynamic viscosity |
| **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 |

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