# BENZO[KL]XANTHENE

**Inchi:** InChI=1S/C16H10O/c1-2-9-14-12(7-1)13-8-3-5-11-6-4-10-15(17-14)16(11)13/h1-10H
**InchiKey:** QKOSFCWXOIAFTO-UHFFFAOYSA-N
**Formula:** C16H10O
**SMILES:** c1ccc2c(c1)Oc1cccc3cccc-2c13
**Mol. weight [g/mol]:** 218.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 154.40 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 30.37 | kJ/mol | Joback Method |
| hvap | 96.86 | kJ/mol | Cheméo Relay (1.0) |
| ie | 7.24 | eV | Cheméo Relay (1.0) |
| log10ws | -6.54 | | Cheméo Relay (1.0) |
| logp | 4.612 | | Crippen Method |
| mcvol | 164.330 | ml/mol | McGowan Method |
| rinpol | 360.96 | | NIST Webbook |
| rinpol | 360.96 | | NIST Webbook |
| rinpol | 361.38 | | NIST Webbook |
| rinpol | 361.60 | | NIST Webbook |
| rinpol | 359.77 | | NIST Webbook |
| rinpol | 361.38 | | NIST Webbook |
| rinpol | 359.85 | | NIST Webbook |
| tb | 651.81 | K | Cheméo Relay (1.0) |
| tf | 371.00 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 416.92 | J/mol×K | 682.58 | Joback Method |
| cpg | 430.22 | J/mol×K | 725.98 | Joback Method |
| cpg | 442.41 | J/mol×K | 769.39 | Joback Method |
| cpg | 453.69 | J/mol×K | 812.79 | Joback Method |
| cpg | 464.27 | J/mol×K | 856.19 | Joback Method |
| cpg | 474.35 | J/mol×K | 899.59 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 484.13 | J/mol×K | 943.00 | Joback Method |
| dvisc | 0.0020931 | Pa×s | 448.97 | Joback Method |
| dvisc | 0.0017633 | Pa×s | 487.91 | Joback Method |
| dvisc | 0.0015236 | Pa×s | 526.84 | Joback Method |
| dvisc | 0.0013433 | Pa×s | 565.77 | Joback Method |
| dvisc | 0.0012037 | Pa×s | 604.71 | Joback Method |
| dvisc | 0.0010930 | Pa×s | 643.64 | Joback Method |
| dvisc | 0.0010034 | Pa×s | 682.58 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C200237&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# Legend

**cpg:** Ideal gas heat capacity

**dvisc:** Dynamic viscosity

**hf:** Enthalpy of formation at standard conditions

**hfus:** Enthalpy of fusion at standard conditions

**hvap:** Enthalpy of vaporization at standard conditions

**ie:** Ionization energy

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

**tb:** Normal Boiling Point Temperature

**tf:** Normal melting (fusion) point