# 3-Bromobenzanthrone

**Other names:** 7H-Benz[de]anthracen-7-one, 3-bromo-
Benzanthrone, 3-bromo-
3-Bromobenz[de]anthrone
7-Bromomesobenzanthrone
3-Brombenzanthrone
3-Bromo-7H-benz(de)anthracen-7-one
7H-Benz[de]anthracene-7-one, 3-bromo-
3-Bromo-7H-benzo[de]anthracen-7-one
NSC 13976
3-bromobenz[de]anthracen-7-one

**Inchi:** InChI=1S/C17H9BrO/c18-15-9-8-11-10-4-1-2-5-12(10)17(19)14-7-3-6-13(15)16(11)14/h1

**InchiKey:** WVECFEIAZAKUNF-UHFFFAOYSA-N

**Formula:** C17H9BrO

**SMILES:** O=C1c2ccccc2-c2ccc(Br)c3cccc1c23

**Mol. weight [g/mol]:** 309.16

**CAS:** 81-96-9

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 369.60 | kJ/mol | Joback Method |
| hf | 218.13 | kJ/mol | Joback Method |
| hfus | 29.39 | kJ/mol | Joback Method |
| hvap | 72.84 | kJ/mol | Joback Method |
| ie | 8.50 | eV | NIST Webbook |
| log10ws | -7.25 | | Crippen Method |
| logp | 4.814 | | Crippen Method |
| mcvol | 191.620 | ml/mol | McGowan Method |
| pc | 3135.00 | kPa | Joback Method |
| tb | 817.47 | K | Joback Method |
| tc | 1096.44 | K | Joback Method |
| tf | 446.35 ± 0.30 | K | NIST Webbook |
| tf | 449.75 ± 0.35 | K | NIST Webbook |
| tf | 450.45 ± 0.25 | K | NIST Webbook |
| tf | 445.65 ± 0.50 | K | NIST Webbook |
| vc | 0.737 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 489.72 | J/mol×K | 817.47 | Joback Method |
| cpg | 501.89 | J/mol×K | 863.96 | Joback Method |
| cpg | 513.35 | J/mol×K | 910.46 | Joback Method |
| cpg | 524.27 | J/mol×K | 956.95 | Joback Method |
| cpg | 534.88 | J/mol×K | 1003.45 | Joback Method |
| cpg | 545.36 | J/mol×K | 1049.94 | Joback Method |
| cpg | 555.92 | J/mol×K | 1096.44 | Joback Method |

# Sources

| | |
|---|---|
| **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=C81969&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **ie:** | Ionization energy |
| **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 |