# «alpha»-Bromomesitylene

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|---|---|
| **Other names:** | 1-(Bromomethyl)-3,5-dimethylbenzene |
| | 3,5-Dimethylbenzyl bromide |
| | Benzene, 1-(bromomethyl)-3,5-dimethyl- |
| | alpha-Bromomesitylene |
| **Inchi:** | InChI=1S/C9H11Br/c1-7-3-8(2)5-9(4-7)6-10/h3-5H,6H2,1-2H3 |
| **InchiKey:** | QXDHXCVJGBTQMK-UHFFFAOYSA-N |
| **Formula:** | C9H11Br |
| **SMILES:** | Cc1cc(C)cc(CBr)c1 |
| **Mol. weight [g/mol]:** | 199.09 |
| **CAS:** | 27129-86-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 132.37 | kJ/mol | Joback Method |
| hf | 10.83 | kJ/mol | Joback Method |
| hfus | 17.61 | kJ/mol | Joback Method |
| hvap | 45.66 | kJ/mol | Joback Method |
| log10ws | -3.73 | | Crippen Method |
| logp | 3.198 | | Crippen Method |
| mcvol | 131.410 | ml/mol | McGowan Method |
| pc | 3411.87 | kPa | Joback Method |
| tb | 508.12 | K | Joback Method |
| tc | 735.27 | K | Joback Method |
| tf | 302.45 | K | Joback Method |
| vc | 0.493 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 254.57 | J/mol×K | 508.12 | Joback Method |
| cpg | 309.79 | J/mol×K | 697.41 | Joback Method |
| cpg | 300.10 | J/mol×K | 659.55 | Joback Method |
| cpg | 289.77 | J/mol×K | 621.70 | Joback Method |
| cpg | 278.77 | J/mol×K | 583.84 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 267.04 | J/mol×K | 545.98 | Joback Method |
| cpg | 318.86 | J/mol×K | 735.27 | Joback Method |
| dvisc | 0.0002613 | Pa×s | 508.12 | Joback Method |
| dvisc | 0.0003177 | Pa×s | 473.84 | Joback Method |
| dvisc | 0.0003983 | Pa×s | 439.56 | Joback Method |
| dvisc | 0.0005187 | Pa×s | 405.28 | Joback Method |
| dvisc | 0.0007095 | Pa×s | 371.01 | Joback Method |
| dvisc | 0.0010342 | Pa×s | 336.73 | Joback Method |
| dvisc | 0.0016421 | Pa×s | 302.45 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 382.50 ± 1.50 | K | 2.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.44935e+01 |
| Coeff. B | -4.12674e+03 |
| Coeff. C | -8.10260e+01 |
| Temperature range (K), min. | 371.52 |
| Temperature range (K), max. | 530.46 |

# 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=C27129868&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**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 |
| **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 |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |