# 4-Penten-2-ol, dibromoacetate

**Inchi:** InChI=1S/C7H10Br2O2/c1-3-4-5(2)11-7(10)6(8)9/h3,5-6H,1,4H2,2H3
**InchiKey:** JQTBJKRYXSYYEA-UHFFFAOYSA-N
**Formula:** C7H10Br2O2
**SMILES:** C=CCC(C)OC(=O)C(Br)Br
**Mol. weight [g/mol]:** 285.96

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -114.26 | kJ/mol | Joback Method |
| hf | -265.08 | kJ/mol | Joback Method |
| hfus | 18.92 | kJ/mol | Joback Method |
| hvap | 51.76 | kJ/mol | Joback Method |
| log10ws | -3.05 | | Crippen Method |
| logp | 2.610 | | Crippen Method |
| mcvol | 147.630 | ml/mol | McGowan Method |
| pc | 3682.02 | kPa | Joback Method |
| rinpol | 1241.00 | | NIST Webbook |
| rinpol | 1241.00 | | NIST Webbook |
| ripol | 1784.00 | | NIST Webbook |
| ripol | 1784.00 | | NIST Webbook |
| tb | 563.97 | K | Joback Method |
| tc | 783.27 | K | Joback Method |
| tf | 328.65 | K | Joback Method |
| vc | 0.544 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 293.26 | J/mol×K | 563.97 | Joback Method |
| cpg | 337.62 | J/mol×K | 746.72 | Joback Method |
| cpg | 329.88 | J/mol×K | 710.17 | Joback Method |
| cpg | 321.60 | J/mol×K | 673.62 | Joback Method |
| cpg | 312.75 | J/mol×K | 637.07 | Joback Method |
| cpg | 303.32 | J/mol×K | 600.52 | Joback Method |

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|---|---|---|---|---|
| cpg | 344.85 | J/mol×K | 783.27 | Joback Method |
| dvisc | 0.0002529 | Pa×s | 563.97 | Joback Method |
| dvisc | 0.0003261 | Pa×s | 524.75 | Joback Method |
| dvisc | 0.0004381 | Pa×s | 485.53 | Joback Method |
| dvisc | 0.0006199 | Pa×s | 446.31 | Joback Method |
| dvisc | 0.0009378 | Pa×s | 407.09 | Joback Method |
| dvisc | 0.0015497 | Pa×s | 367.87 | Joback Method |
| dvisc | 0.0028871 | Pa×s | 328.65 | 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=R26550&Units=SI

# 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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume