# Propanoic acid, 2,3-dibromo, 4-methylpentyl ester

**Inchi:** InChI=1S/C9H16Br2O2/c1-7(2)4-3-5-13-9(12)8(11)6-10/h7-8H,3-6H2,1-2H3
**InchiKey:** RERWDLPVFANPHQ-UHFFFAOYSA-N
**Formula:** C9H16Br2O2
**SMILES:** CC(C)CCCOC(=O)C(Br)CBr
**Mol. weight [g/mol]:** 316.03

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -185.26 | kJ/mol | Joback Method |
| hf | -431.79 | kJ/mol | Joback Method |
| hfus | 25.38 | kJ/mol | Joback Method |
| hvap | 56.88 | kJ/mol | Joback Method |
| log10ws | -3.19 | | Crippen Method |
| logp | 3.124 | | Crippen Method |
| mcvol | 180.110 | ml/mol | McGowan Method |
| pc | 2823.32 | kPa | Joback Method |
| rinpol | 1474.00 | | NIST Webbook |
| rinpol | 1474.00 | | NIST Webbook |
| tb | 613.05 | K | Joback Method |
| tc | 820.85 | K | Joback Method |
| tf | 352.95 | K | Joback Method |
| vc | 0.675 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 405.74 | J/mol×K | 613.05 | Joback Method |
| cpg | 461.72 | J/mol×K | 786.22 | Joback Method |
| cpg | 451.83 | J/mol×K | 751.58 | Joback Method |
| cpg | 441.31 | J/mol×K | 716.95 | Joback Method |
| cpg | 430.13 | J/mol×K | 682.32 | Joback Method |
| cpg | 418.29 | J/mol×K | 647.68 | Joback Method |
| cpg | 471.01 | J/mol×K | 820.85 | Joback Method |
| dvisc | 0.0001885 | Pa×s | 613.05 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002468 | Pa×s | 569.70 | Joback Method |
| dvisc | 0.0003379 | Pa×s | 526.35 | Joback Method |
| dvisc | 0.0004893 | Pa×s | 483.00 | Joback Method |
| dvisc | 0.0007622 | Pa×s | 439.65 | Joback Method |
| dvisc | 0.0013082 | Pa×s | 396.30 | Joback Method |
| dvisc | 0.0025642 | Pa×s | 352.95 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R30200&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 |

# Legend

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|---|---|
| **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 |