# 5-bromovaleric acid, 3-methylbut-2-enyl ester

**Inchi:** InChI=1S/C10H17BrO2/c1-9(2)6-8-13-10(12)5-3-4-7-11/h6H,3-5,7-8H2,1-2H3
**InchiKey:** KMNWYBWUEWICRT-UHFFFAOYSA-N
**Formula:** C10H17BrO2
**SMILES:** CC(C)=CCOC(=O)CCCCBr
**Mol. weight [g/mol]:** 249.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 28.62 | kJ/mol | Joback Method |
| log10ws | -3.46 | | Cheméo Relay (1.0) |
| logp | 3.061 | | Crippen Method |
| mcvol | 172.400 | ml/mol | McGowan Method |
| rinpol | 1544.90 | | NIST Webbook |
| tb | 533.41 | K | Cheméo Relay (1.0) |
| tc | 707.94 | K | Cheméo Relay (1.0) |
| tf | 250.80 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 393.28 | J/mol×K | 574.69 | Joback Method |
| cpg | 406.57 | J/mol×K | 607.39 | Joback Method |
| cpg | 419.19 | J/mol×K | 640.10 | Joback Method |
| cpg | 431.15 | J/mol×K | 672.80 | Joback Method |
| cpg | 442.49 | J/mol×K | 705.51 | Joback Method |
| cpg | 453.24 | J/mol×K | 738.21 | Joback Method |
| cpg | 463.41 | J/mol×K | 770.92 | Joback Method |

## Sources

**Cheméo Relay (1.0):**

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|---|---|
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U292563&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **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 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |