# Propanoic acid, 3-bromo, 3-methylbutyl ester

**Other names:** Propanoic acid, 3-bromo, isopentyl ester
**Inchi:** InChI=1S/C8H15BrO2/c1-7(2)4-6-11-8(10)3-5-9/h7H,3-6H2,1-2H3
**InchiKey:** AIAZLKUDLPPYBB-UHFFFAOYSA-N
**Formula:** C8H15BrO2
**SMILES:** CC(C)CCOC(=O)CCBr
**Mol. weight [g/mol]:** 223.11
**CAS:** 100983-12-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -205.56 | kJ/mol | Joback Method |
| hf | -432.20 | kJ/mol | Joback Method |
| hfus | 21.02 | kJ/mol | Joback Method |
| hvap | 48.61 | kJ/mol | Joback Method |
| log10ws | -2.22 | | Crippen Method |
| logp | 2.361 | | Crippen Method |
| mcvol | 148.520 | ml/mol | McGowan Method |
| pc | 2881.21 | kPa | Joback Method |
| rinpol | 1236.00 | | NIST Webbook |
| rinpol | 1236.00 | | NIST Webbook |
| ripol | 1687.00 | | NIST Webbook |
| tb | 524.45 | K | Joback Method |
| tc | 718.18 | K | Joback Method |
| tf | 296.88 | K | Joback Method |
| vc | 0.564 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 320.63 | J/mol×K | 524.45 | Joback Method |
| cpg | 332.86 | J/mol×K | 556.74 | Joback Method |
| cpg | 344.53 | J/mol×K | 589.03 | Joback Method |
| cpg | 355.66 | J/mol×K | 621.31 | Joback Method |
| cpg | 366.25 | J/mol×K | 653.60 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 376.32 | J/mol×K | 685.89 | Joback Method |
| cpg | 385.87 | J/mol×K | 718.18 | Joback Method |
| dvisc | 0.0033286 | Pa×s | 296.88 | Joback Method |
| dvisc | 0.0017041 | Pa×s | 334.81 | Joback Method |
| dvisc | 0.0009998 | Pa×s | 372.74 | Joback Method |
| dvisc | 0.0006473 | Pa×s | 410.67 | Joback Method |
| dvisc | 0.0004510 | Pa×s | 448.59 | Joback Method |
| dvisc | 0.0003325 | Pa×s | 486.52 | Joback Method |
| dvisc | 0.0002562 | Pa×s | 524.45 | 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=C100983128&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

Latest version available from: