# 2- Bromopropionic acid, tridecyl ester

**Inchi:** InChI=1S/C16H31BrO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-19-16(18)15(2)17/h15H,3-14H2
**InchiKey:** VLVJDJNDVAPFNI-UHFFFAOYSA-N
**Formula:** C16H31BrO2
**SMILES:** CCCCCCCCCCCCCOC(=O)C(C)Br
**Mol. weight [g/mol]:** 335.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -138.20 | kJ/mol | Joback Method |
| hf | -597.32 | kJ/mol | Joback Method |
| hfus | 41.74 | kJ/mol | Joback Method |
| hvap | 66.41 | kJ/mol | Joback Method |
| log10ws | -5.93 | | Crippen Method |
| logp | 5.624 | | Crippen Method |
| mcvol | 261.240 | ml/mol | McGowan Method |
| pc | 1444.64 | kPa | Joback Method |
| rinpol | 2056.30 | | NIST Webbook |
| rinpol | 2056.30 | | NIST Webbook |
| tb | 707.49 | K | Joback Method |
| tc | 888.41 | K | Joback Method |
| tf | 387.04 | K | Joback Method |
| vc | 1.012 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 729.06 | J/mol×K | 707.49 | Joback Method |
| cpg | 806.28 | J/mol×K | 858.25 | Joback Method |
| cpg | 792.42 | J/mol×K | 828.10 | Joback Method |
| cpg | 777.79 | J/mol×K | 797.95 | Joback Method |
| cpg | 762.37 | J/mol×K | 767.80 | Joback Method |
| cpg | 746.14 | J/mol×K | 737.64 | Joback Method |
| cpg | 819.40 | J/mol×K | 888.41 | Joback Method |
| dvisc | 0.0000956 | Pa×s | 707.49 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001277 | Pa×s | 654.08 | Joback Method |
| dvisc | 0.0001796 | Pa×s | 600.67 | Joback Method |
| dvisc | 0.0002699 | Pa×s | 547.26 | Joback Method |
| dvisc | 0.0004431 | Pa×s | 493.86 | Joback Method |
| dvisc | 0.0008202 | Pa×s | 440.45 | Joback Method |
| dvisc | 0.0017995 | Pa×s | 387.04 | Joback Method |

# Sources

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|---|---|
| **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=U292439&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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