# 2- Bromopropionic acid, octadecyl ester

**Inchi:** InChI=1S/C21H41BrO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-21(23)20(2)
**InchiKey:** KPORSMDXMDNWRZ-UHFFFAOYSA-N
**Formula:** C21H41BrO2
**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)C(C)Br
**Mol. weight [g/mol]:** 405.45
**CAS:** 89876-55-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -96.10 | kJ/mol | Joback Method |
| hf | -700.52 | kJ/mol | Joback Method |
| hfus | 54.70 | kJ/mol | Joback Method |
| hvap | 77.54 | kJ/mol | Joback Method |
| log10ws | -8.02 | | Crippen Method |
| logp | 7.575 | | Crippen Method |
| mcvol | 331.690 | ml/mol | McGowan Method |
| pc | 1033.24 | kPa | Joback Method |
| rinpol | 2548.60 | | NIST Webbook |
| tb | 821.89 | K | Joback Method |
| tc | 1009.13 | K | Joback Method |
| tf | 443.39 | K | Joback Method |
| vc | 1.292 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1024.62 | J/mol×K | 821.89 | Joback Method |
| cpg | 1043.63 | J/mol×K | 853.10 | Joback Method |
| cpg | 1061.60 | J/mol×K | 884.30 | Joback Method |
| cpg | 1078.58 | J/mol×K | 915.51 | Joback Method |
| cpg | 1094.61 | J/mol×K | 946.72 | Joback Method |
| cpg | 1109.71 | J/mol×K | 977.92 | Joback Method |
| cpg | 1123.94 | J/mol×K | 1009.13 | Joback Method |
| dvisc | 0.0010210 | Pa×s | 443.39 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004422 | Pa×s | 506.47 | Joback Method |
| dvisc | 0.0002305 | Pa×s | 569.56 | Joback Method |
| dvisc | 0.0001368 | Pa×s | 632.64 | Joback Method |
| dvisc | 0.0000893 | Pa×s | 695.72 | Joback Method |
| dvisc | 0.0000626 | Pa×s | 758.81 | Joback Method |
| dvisc | 0.0000463 | Pa×s | 821.89 | Joback Method |

# Sources

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|---|---|
| **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=C89876551&Units=SI |
| **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 |
| **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 |