# Homocysteine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

**Inchi:** InChI=1S/C15H27NO6S/c1-6-20-14(18)16-12(8-9-23-15(19)21-7-2)13(17)22-11(5)10(3)4

**InchiKey:** USMTUXCTEQBQQN-JHJMLUEUSA-N

**Formula:** C15H27NO6S

**SMILES:** CCOC(=O)NC(CCSC(=O)OCC)C(=O)OC(C)C(C)C

**Mol. weight [g/mol]:** 349.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -511.15 | kJ/mol | Joback Method |
| hf | -1007.83 | kJ/mol | Joback Method |
| hfus | 41.63 | kJ/mol | Joback Method |
| hvap | 88.54 | kJ/mol | Joback Method |
| log10ws | -3.70 | | Crippen Method |
| logp | 2.969 | | Crippen Method |
| mcvol | 270.860 | ml/mol | McGowan Method |
| pc | 1644.42 | kPa | Joback Method |
| rinpol | 2188.40 | | NIST Webbook |
| rinpol | 2197.30 | | NIST Webbook |
| rinpol | 2188.40 | | NIST Webbook |
| tb | 889.10 | K | Joback Method |
| tc | 1097.41 | K | Joback Method |
| tf | 517.35 | K | Joback Method |
| vc | 1.018 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 843.88 | J/mol×K | 889.10 | Joback Method |
| cpg | 856.88 | J/mol×K | 923.82 | Joback Method |
| cpg | 868.59 | J/mol×K | 958.54 | Joback Method |
| cpg | 878.98 | J/mol×K | 993.26 | Joback Method |
| cpg | 888.05 | J/mol×K | 1027.97 | Joback Method |
| cpg | 895.78 | J/mol×K | 1062.69 | Joback Method |
| cpg | 902.18 | J/mol×K | 1097.41 | Joback Method |

# Sources

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|---|---|
| **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=R501727&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |