# (Octadecyl E)-2-methylbut-2-enoate

**Inchi:** InChI=1S/C23H44O2/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-23(24)22(3
**InchiKey:** SBKJWIXXZKMGTM-RREIPUBJSA-N
**Formula:** C23H44O2
**SMILES:** CC=C(C)C(=O)OCCCCCCCCCCCCCCCCCC
**Mol. weight [g/mol]:** 352.59

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -19.47 | kJ/mol | Joback Method |
| hf | -655.42 | kJ/mol | Joback Method |
| hfus | 57.01 | kJ/mol | Joback Method |
| hvap | 75.99 | kJ/mol | Joback Method |
| log10ws | -8.17 | | Crippen Method |
| logp | 7.757 | | Crippen Method |
| mcvol | 338.070 | ml/mol | McGowan Method |
| pc | 905.61 | kPa | Joback Method |
| rinpol | 2535.00 | | NIST Webbook |
| rinpol | 2535.00 | | NIST Webbook |
| tb | 805.97 | K | Joback Method |
| tc | 988.62 | K | Joback Method |
| tf | 402.09 | K | Joback Method |
| vc | 1.329 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1068.44 | J/mol×K | 805.97 | Joback Method |
| cpg | 1088.98 | J/mol×K | 836.41 | Joback Method |
| cpg | 1108.48 | J/mol×K | 866.85 | Joback Method |
| cpg | 1126.99 | J/mol×K | 897.30 | Joback Method |
| cpg | 1144.53 | J/mol×K | 927.74 | Joback Method |
| cpg | 1161.16 | J/mol×K | 958.18 | Joback Method |
| cpg | 1176.91 | J/mol×K | 988.62 | 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=U373757&Units=SI |

# 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 |

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