# Ethylene brassylate

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|---|---|
| **Other names:** | 1,4-Dioxacycloheptadecane-5,17-dione |
| | Astratone |
| | Ethylene undecane dicarboxylate |
| | Musk T |
| | Tridecanedioic acid, cyclic ethylene ester |
| | 1,11-Undecanedicarboxylic acid, ester with ethylene glycol |
| | Emeressence 1150 |
| **Inchi:** | InChI=1S/C15H26O4/c16-14-10-8-6-4-2-1-3-5-7-9-11-15(17)19-13-12-18-14/h1-13H2 |
| **InchiKey:** | XRHCAGNSDHCHFJ-UHFFFAOYSA-N |
| **Formula:** | C15H26O4 |
| **SMILES:** | O=C1CCCCCCCCCCCC(=O)OCCO1 |
| **Mol. weight [g/mol]:** | 270.36 |
| **CAS:** | 105-95-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -442.94 | kJ/mol | Joback Method |
| hf | -885.43 | kJ/mol | Joback Method |
| hfus | 17.25 | kJ/mol | Joback Method |
| hvap | 69.13 | kJ/mol | Joback Method |
| log10ws | -3.72 | | Crippen Method |
| logp | 3.377 | | Crippen Method |
| mcvol | 226.230 | ml/mol | McGowan Method |
| pc | 2282.77 | kPa | Joback Method |
| rinpol | 1988.60 | | NIST Webbook |
| tb | 803.33 | K | Joback Method |
| tc | 1084.74 | K | Joback Method |
| tf | 421.29 | K | Joback Method |
| vc | 0.777 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 748.62 | J/mol×K | 803.33 | Joback Method |

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|---|---|---|---|---|
| cpg | 773.82 | J/mol×K | 850.23 | Joback Method |
| cpg | 795.34 | J/mol×K | 897.13 | Joback Method |
| cpg | 812.93 | J/mol×K | 944.03 | Joback Method |
| cpg | 826.38 | J/mol×K | 990.94 | Joback Method |
| cpg | 835.45 | J/mol×K | 1037.84 | Joback Method |
| cpg | 839.93 | J/mol×K | 1084.74 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C105953&Units=SI |
| **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 |

# Legend

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|---|---|
| **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 |