# «gamma»-Asarone

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|---|---|
| **Other names:** | Isoasarone |
| | euasarone |
| | Benzene, 1-(2-propenyl)-2,4,5-trimethoxy |
| | 2,4,5-Trimethoxy-allylbenzene |
| **Inchi:** | InChI=1S/C12H16O3/c1-5-6-9-7-11(14-3)12(15-4)8-10(9)13-2/h5,7-8H,1,6H2,2-4H3 |
| **InchiKey:** | AUNAUZZQBAIQFJ-UHFFFAOYSA-N |
| **Formula:** | C12H16O3 |
| **SMILES:** | C=CCc1cc(OC)c(OC)cc1OC |
| **Mol. weight [g/mol]:** | 208.25 |
| **CAS:** | 5353-15-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -93.48 | kJ/mol | Joback Method |
| hf | -360.12 | kJ/mol | Joback Method |
| hfus | 21.99 | kJ/mol | Joback Method |
| hvap | 53.13 | kJ/mol | Joback Method |
| log10ws | -2.91 | | Crippen Method |
| logp | 2.441 | | Crippen Method |
| mcvol | 169.490 | ml/mol | McGowan Method |
| pc | 2282.77 | kPa | Joback Method |
| rinpol | 1535.00 | | NIST Webbook |
| rinpol | 1533.00 | | NIST Webbook |
| rinpol | 1535.00 | | NIST Webbook |
| rinpol | 1574.00 | | NIST Webbook |
| rinpol | 1536.00 | | NIST Webbook |
| rinpol | 1578.50 | | NIST Webbook |
| ripol | 2261.00 | | NIST Webbook |
| ripol | 2263.00 | | NIST Webbook |
| ripol | 2261.00 | | NIST Webbook |
| tb | 579.52 | K | Joback Method |
| tc | 780.79 | K | Joback Method |
| tf | 353.91 | K | Joback Method |
| vc | 0.634 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 404.13 | J/mol×K | 579.52 | Joback Method |
| cpg | 470.12 | J/mol×K | 747.24 | Joback Method |
| cpg | 458.19 | J/mol×K | 713.70 | Joback Method |
| cpg | 445.60 | J/mol×K | 680.15 | Joback Method |
| cpg | 432.39 | J/mol×K | 646.61 | Joback Method |
| cpg | 418.56 | J/mol×K | 613.06 | Joback Method |
| cpg | 481.39 | J/mol×K | 780.79 | Joback Method |
| dvisc | 0.0001098 | Pa×s | 579.52 | Joback Method |
| dvisc | 0.0001333 | Pa×s | 541.92 | Joback Method |
| dvisc | 0.0001666 | Pa×s | 504.32 | Joback Method |
| dvisc | 0.0002159 | Pa×s | 466.72 | Joback Method |
| dvisc | 0.0002927 | Pa×s | 429.11 | Joback Method |
| dvisc | 0.0004207 | Pa×s | 391.51 | Joback Method |
| dvisc | 0.0006532 | Pa×s | 353.91 | 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=C5353151&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |