# Isonovalal

**Inchi:** InChI=1S/C10H16O/c1-8(2)10(4)6-5-9(3)7-11/h5,7-8H,4,6H2,1-3H3/b9-5-
**InchiKey:** KDMDLRXLBMMBSU-UITAMQMPSA-N
**Formula:** C10H16O
**SMILES:** C=C(CC=C(C)C=O)C(C)C
**Mol. weight [g/mol]:** 152.23
**CAS:** 112164-19-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 82.32 | kJ/mol | Joback Method |
| hf | -117.52 | kJ/mol | Joback Method |
| hfus | 16.72 | kJ/mol | Joback Method |
| hvap | 43.63 | kJ/mol | Joback Method |
| log10ws | -2.75 | | Crippen Method |
| logp | 2.734 | | Crippen Method |
| mcvol | 144.730 | ml/mol | McGowan Method |
| pc | 2520.12 | kPa | Joback Method |
| rinpol | 1169.00 | | NIST Webbook |
| rinpol | 1169.00 | | NIST Webbook |
| tb | 477.02 | K | Joback Method |
| tc | 667.36 | K | Joback Method |
| tf | 194.70 | K | Joback Method |
| vc | 0.570 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 308.54 | J/mol×K | 477.02 | Joback Method |
| cpg | 322.55 | J/mol×K | 508.74 | Joback Method |
| cpg | 335.84 | J/mol×K | 540.47 | Joback Method |
| cpg | 348.43 | J/mol×K | 572.19 | Joback Method |
| cpg | 360.36 | J/mol×K | 603.91 | Joback Method |
| cpg | 371.65 | J/mol×K | 635.63 | Joback Method |
| cpg | 382.35 | J/mol×K | 667.36 | Joback Method |

# Sources

| | |
|---|---|
| **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=C112164199&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 |
| **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 |