

trans-«beta»-Ionone

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| Other names: | 3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (E)- (E)-«beta»-Ionone 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one «beta»-E-Ionone [E]-4-[2,6,6-trimethyl-1-cyclohexen-1-yl]-3-buten-2-one 3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (3E)- «beta»-Ionone «beta»-Ionone (E)-4-(2,6,6-Trimethylcyclohexen-1-yl)-3-buten-2-one (3E)-4-(2,6,6-trimethylcyclohex-1-enyl)-3-buten-2-one (dihydro-«beta»-ionone) |
| Inchi: | InChI=1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h7-8H,5-6,9H2,1-4H3/b8-7+ |
| InchiKey: | PSQYTAPXSHCGMF-BQYQJAHWSA-N |
| Formula: | C13H20O |
| SMILES: | CC(=O)C=CC1=C(C)CCCC1(C)C |
| Mol. weight [g/mol]: | 192.30 |
| CAS: | 79-77-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|--------|----------------|
| chl | -7712.40 ± 3.50 | kJ/mol | NIST Webbook |
| gf | 39.54 | kJ/mol | Joback Method |
| hf | -202.61 | kJ/mol | Joback Method |
| hfl | -261.50 ± 3.50 | kJ/mol | NIST Webbook |
| hfus | 17.21 | kJ/mol | Joback Method |
| hvap | 52.13 | kJ/mol | Joback Method |
| log10ws | -3.90 | | Crippen Method |
| logp | 3.658 | | Crippen Method |
| mcvol | 176.140 | ml/mol | McGowan Method |
| pc | 2278.41 | kPa | Joback Method |
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| tb | 583.78 | K | Joback Method |
| tc | 802.88 | K | Joback Method |
| tf | 338.20 | K | Joback Method |
| vc | 0.666 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 437.25 | J/mol×K | 583.78 | Joback Method |
| cpg | 455.12 | J/mol×K | 620.30 | Joback Method |
| cpg | 471.95 | J/mol×K | 656.81 | Joback Method |
| cpg | 487.87 | J/mol×K | 693.33 | Joback Method |
| cpg | 503.02 | J/mol×K | 729.85 | Joback Method |
| cpg | 517.51 | J/mol×K | 766.36 | Joback Method |
| cpg | 531.49 | J/mol×K | 802.88 | Joback Method |
| cpl | 388.40 | J/mol×K | 313.60 | NIST Webbook |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 400.20 | K | 1.60 | NIST Webbook |

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Legend

| | |
|-----------------|---|
| chl: | Standard liquid enthalpy of combustion |
| cpg: | Ideal gas heat capacity |
| cpl: | Liquid phase heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfl: | Liquid phase enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcpvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |

tf: Normal melting (fusion) point

vc: Critical Volume

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