

endo-Tricyclo[6,2,1,0(2,6)]dec-3-en-8-«beta»-ol,

Inchi:
acetate

InChI=1S/C12H16O2/c1-7(13)14-12-6-8-5-11(12)10-4-2-3-9(8)10/h2-3,8-12H,4-6H2,1H3

InchiKey:

RGVQNSFGUOIKFF-SEIUWDOFSA-N

Formula:

C12H16O2

SMILES:

CC(=O)OC1CC2CC1C1CC=CC21

Mol. weight [g/mol]:

192.25

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 0.93 | kJ/mol | Joback Method |
| hf | -306.47 | kJ/mol | Joback Method |
| hfus | 25.29 | kJ/mol | Joback Method |
| hvap | 51.05 | kJ/mol | Joback Method |
| log10ws | -2.39 | | Crippen Method |
| logp | 2.150 | | Crippen Method |
| mcvol | 150.500 | ml/mol | McGowan Method |
| pc | 2659.77 | kPa | Joback Method |
| rinpol | 1401.00 | | NIST Webbook |
| ripol | 1870.00 | | NIST Webbook |
| tb | 564.56 | K | Joback Method |
| tc | 780.81 | K | Joback Method |
| tf | 339.74 | K | Joback Method |
| vc | 0.579 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 407.03 | J/molxK | 564.56 | Joback Method |
| cpg | 425.84 | J/molxK | 600.60 | Joback Method |
| cpg | 443.41 | J/molxK | 636.64 | Joback Method |
| cpg | 459.82 | J/molxK | 672.68 | Joback Method |
| cpg | 475.14 | J/molxK | 708.72 | Joback Method |
| cpg | 489.45 | J/molxK | 744.76 | Joback Method |
| cpg | 502.84 | J/molxK | 780.81 | Joback Method |
| dvisc | 0.0018650 | Paxs | 339.74 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0019297 | Paxs | 377.21 | Joback Method |
| dvisc | 0.0019844 | Paxs | 414.68 | Joback Method |
| dvisc | 0.0020312 | Paxs | 452.15 | Joback Method |
| dvisc | 0.0020717 | Paxs | 489.62 | Joback Method |
| dvisc | 0.0021070 | Paxs | 527.09 | Joback Method |
| dvisc | 0.0021382 | Paxs | 564.56 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=R386157&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 |

Latest version available from:

<https://www.chemeo.com/cid/19-573-5/endo-Tricyclo-6-2-1-0-2-6-dec-3-en-8-beta-ol-acetate.pdf>

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