

Tricyclo[8.4.0.0(2,7)]dodecane, isomer # 2

Inchi: InChI=1S/C14H24/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h11-14H,1-10H2
InchiKey: GNMCGMFNBARSIIY-UHFFFAOYSA-N
Formula: C14H24
SMILES: C1CCC2C(C1)CCC1CCCCC12
Mol. weight [g/mol]: 192.34

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 181.04 | kJ/mol | Joback Method |
| hf | -165.03 | kJ/mol | Joback Method |
| hfus | 16.99 | kJ/mol | Joback Method |
| hvap | 47.05 | kJ/mol | Joback Method |
| log10ws | -4.40 | | Crippen Method |
| logp | 4.393 | | Crippen Method |
| mcvol | 175.540 | ml/mol | McGowan Method |
| pc | 2311.39 | kPa | Joback Method |
| rinpol | 1513.00 | | NIST Webbook |
| rinpol | 1538.00 | | NIST Webbook |
| ripol | 1747.00 | | NIST Webbook |
| ripol | 1705.00 | | NIST Webbook |
| tb | 556.62 | K | Joback Method |
| tc | 789.03 | K | Joback Method |
| tf | 279.52 | K | Joback Method |
| vc | 0.649 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 476.02 | J/molxK | 556.62 | Joback Method |
| cpg | 503.38 | J/molxK | 595.35 | Joback Method |
| cpg | 528.90 | J/molxK | 634.09 | Joback Method |
| cpg | 552.65 | J/molxK | 672.82 | Joback Method |
| cpg | 574.73 | J/molxK | 711.56 | Joback Method |
| cpg | 595.25 | J/molxK | 750.29 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 614.30 | J/molxK | 789.03 | Joback Method |
| dvisc | 0.0033535 | Paxs | 279.52 | Joback Method |
| dvisc | 0.0021240 | Paxs | 325.70 | Joback Method |
| dvisc | 0.0015068 | Paxs | 371.89 | Joback Method |
| dvisc | 0.0011532 | Paxs | 418.07 | Joback Method |
| dvisc | 0.0009308 | Paxs | 464.25 | Joback Method |
| dvisc | 0.0007810 | Paxs | 510.44 | Joback Method |
| dvisc | 0.0006747 | Paxs | 556.62 | 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=R524671&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307i |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |

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<https://www.chemeo.com/cid/57-996-4/Tricyclo-8-4-0-0-2-7-dodecane-isomer-2.pdf>

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