

trans-(+)-Bicyclo-[6.1.0]nonane

Inchi: InChI=1S/C9H16/c1-2-4-6-9-7-8(9)5-3-1/h8-9H,1-7H2/t8-,9-/m1/s1
InchiKey: FYECUAIUGWFPJF-RKDXNWHRSA-N
Formula: C9H16
SMILES: C1CCCC2CC2CC1
Mol. weight [g/mol]: 124.22
CAS: 39124-79-3

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|----------------------|----------------|
| chl | -5760.32 ± 0.92 | kJ/mol | NIST Webbook |
| gf | 110.10 | kJ/mol | Joback Method |
| hf | -18.80 ± 1.10 | kJ/mol | NIST Webbook |
| hf | -39.70 ± 3.30 | kJ/mol | NIST Webbook |
| hfl | -82.40 ± 3.20 | kJ/mol | NIST Webbook |
| hfl | -68.20 ± 1.00 | kJ/mol | NIST Webbook |
| hfus | 9.04 | kJ/mol | Joback Method |
| hvap | 42.70 ± 0.60 | kJ/mol | NIST Webbook |
| hvap | 42.70 | kJ/mol | NIST Webbook |
| hvap | 49.40 ± 0.40 | kJ/mol | NIST Webbook |
| hvap | 49.40 | kJ/mol | NIST Webbook |
| ie | 9.36 | eV | NIST Webbook |
| log10ws | -2.90 | | Crippen Method |
| logp | 2.977 | | Crippen Method |
| mcvol | 115.950 | ml/mol | McGowan Method |
| pc | 3276.53 | kPa | Joback Method |
| tb | 431.61 | K | Joback Method |
| tc | 647.88 | K | Joback Method |
| tf | 216.51 | K | Joback Method |
| vc | 0.429 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 240.94 | J/mol×K | 431.61 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 261.35 | J/mol×K | 467.66 | Joback Method |
| cpg | 280.52 | J/mol×K | 503.70 | Joback Method |
| cpg | 298.50 | J/mol×K | 539.75 | Joback Method |
| cpg | 315.35 | J/mol×K | 575.79 | Joback Method |
| cpg | 331.12 | J/mol×K | 611.84 | Joback Method |
| cpg | 345.88 | J/mol×K | 647.88 | Joback Method |
| dvisc | 0.0026731 | Paxs | 216.51 | Joback Method |
| dvisc | 0.0016168 | Paxs | 252.36 | Joback Method |
| dvisc | 0.0011082 | Paxs | 288.21 | Joback Method |
| dvisc | 0.0008258 | Paxs | 324.06 | Joback Method |
| dvisc | 0.0006525 | Paxs | 359.91 | Joback Method |
| dvisc | 0.0005380 | Paxs | 395.76 | Joback Method |
| dvisc | 0.0004581 | Paxs | 431.61 | 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=C39124793&Units=SI |

Legend

| | |
|-----------------|---|
| chl: | Standard liquid enthalpy of combustion |
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| 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 |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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