

2H-Pyran, tetrahydro, 3-chloro-2-butoxy, # 1

Inchi: InChI=1S/C9H17ClO2/c1-2-3-6-11-9-8(10)5-4-7-12-9/h8-9H,2-7H2,1H3
InchiKey: YVJCTCVZSCULEB-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCCCOC1OCCCC1Cl
Mol. weight [g/mol]: 192.68

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -161.41 | kJ/mol | Joback Method |
| hf | -475.07 | kJ/mol | Joback Method |
| hfus | 25.34 | kJ/mol | Joback Method |
| hvap | 47.05 | kJ/mol | Joback Method |
| log10ws | -2.53 | | Crippen Method |
| logp | 2.547 | | Crippen Method |
| mvol | 150.790 | ml/mol | McGowan Method |
| pc | 2568.89 | kPa | Joback Method |
| rinpol | 1275.00 | | NIST Webbook |
| rinpol | 1275.00 | | NIST Webbook |
| tb | 507.00 | K | Joback Method |
| tc | 709.81 | K | Joback Method |
| tf | 273.05 | K | Joback Method |
| vc | 0.559 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 348.05 | J/molxK | 507.00 | Joback Method |
| cpg | 365.23 | J/molxK | 540.80 | Joback Method |
| cpg | 381.62 | J/molxK | 574.60 | Joback Method |
| cpg | 397.21 | J/molxK | 608.40 | Joback Method |
| cpg | 412.01 | J/molxK | 642.20 | Joback Method |
| cpg | 426.03 | J/molxK | 676.01 | Joback Method |
| cpg | 439.27 | J/molxK | 709.81 | Joback Method |
| dvisc | 0.0036685 | Paxs | 273.05 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0018009 | Paxs | 312.04 | Joback Method |
| dvisc | 0.0010355 | Paxs | 351.03 | Joback Method |
| dvisc | 0.0006650 | Paxs | 390.02 | Joback Method |
| dvisc | 0.0004629 | Paxs | 429.02 | Joback Method |
| dvisc | 0.0003423 | Paxs | 468.01 | Joback Method |
| dvisc | 0.0002651 | Paxs | 507.00 | 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=R90961&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 |
| 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/97-098-7/2H-Pyran-tetrahydro-3-chloro-2-butoxy-1.pdf>

Generated by Cheméo on 2024-04-19 18:15:43.88503456 +0000 UTC m=+15839792.805611876.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.