

Benzyl isocyanate

| | |
|-----------------------------|---|
| Other names: | Benzene, (isocyanatomethyl)- |
| Inchi: | InChI=1S/C8H7NO/c10-7-9-6-8-4-2-1-3-5-8/h1-5H,6H2 |
| InchiKey: | YDNLNVZZTACNJX-UHFFFAOYSA-N |
| Formula: | C8H7NO |
| SMILES: | O=C=NCC1ccccc1 |
| Mol. weight [g/mol]: | 133.15 |
| CAS: | 3173-56-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 22.67 | kJ/mol | Joback Method |
| hvap | 45.21 | kJ/mol | Joback Method |
| log10ws | -6.27 | | Crippen Method |
| logp | 1.522 | | Crippen Method |
| mcvol | 107.070 | ml/mol | McGowan Method |
| pc | 4000.70 | kPa | Joback Method |
| rinpol | 1125.80 | | NIST Webbook |
| rinpol | 1137.00 | | NIST Webbook |
| tb | 475.79 | K | Joback Method |
| tc | 696.70 | K | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|--------|-----------------|--------------|
| hvapt | 42.30 | kJ/mol | 363.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| 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=C3173566&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

| | |
|-----------------|---|
| hf: | Enthalpy of formation 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 |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

Latest version available from:

<https://www.chemeo.com/cid/52-016-6/Benzyl-isocyanate.pdf>

Generated by Cheméo on 2024-03-20 10:48:48.559224689 +0000 UTC m=+13220977.479802059.

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