# 1,4-bis(1-isocyanato-1-methylethyl)benzene

**Inchi:** InChI=1S/C14H16N2O2/c1-13(2,15-9-17)11-5-7-12(8-6-11)14(3,4)16-10-18/h5-8H,1-4H3
**InchiKey:** AGJCSCSSMFRMFQ-UHFFFAOYSA-N
**Formula:** C14H16N2O2
**SMILES:** CC(C)(N=C=O)c1ccc(C(C)(C)N=C=O)cc1
**Mol. weight [g/mol]:** 244.29
**CAS:** 2778-41-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -135.55 | kJ/mol | Joback Method |
| hvap | 66.17 | kJ/mol | Joback Method |
| log10ws | -12.08 | | Crippen Method |
| logp | 2.828 | | Crippen Method |
| mcvol | 198.860 | ml/mol | McGowan Method |
| pc | 2356.49 | kPa | Joback Method |
| tb | 678.26 | K | Joback Method |
| tc | 909.46 | K | Joback Method |
| tf | 353.00 ± 2.00 | K | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cps | 415.00 | J/mol×K | 333.00 | NIST Webbook |
| hvapt | 74.00 | kJ/mol | 400.50 | NIST Webbook |

## 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=C2778418&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

| | |
|---|---|
| **cps:** | Solid phase heat capacity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |