

2-Butenal (E), 2,4,6-trichlorophenyl hydrazone

Inchi: InChI=1S/C10H9Cl3N2/c1-2-3-4-14-15-10-8(12)5-7(11)6-9(10)13/h2-6,15H,1H3/b3-2+,1
InchiKey: AWWLLNNSTTXXNE-BYUCVARHSA-N
Formula: C10H9Cl3N2
SMILES: CC=CC=NNc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 263.55

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 158.08 | kJ/mol | Joback Method |
| hvap | 64.98 | kJ/mol | Joback Method |
| log10ws | -4.80 | | Crippen Method |
| logp | 4.621 | | Crippen Method |
| mcvol | 176.080 | ml/mol | McGowan Method |
| pc | 2395.87 | kPa | Joback Method |
| rinpol | 2026.00 | | NIST Webbook |
| tb | 713.12 | K | Joback Method |
| tc | 958.34 | K | Joback Method |

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=R84990&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf: Enthalpy of formation 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 |

Latest version available from:

<https://www.cheméo.com/cid/24-133-7/2-Butenal-E-2-4-6-trichlorophenyl-hydrazone.pdf>

Generated by Cheméo on 2024-04-27 17:31:44.628768755 +0000 UTC m=+16528353.549346066.

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