

1,2-Naphthalenedione, 1-[(4-methylphenyl)hydrazone]-

Inchi: InChI=1S/C17H14N2O/c1-12-6-9-14(10-7-12)18-19-17-15-5-3-2-4-13(15)8-11-16(17)20/
InchiKey: BFBIARQFJLYFRD-ZPHPHTNESA-N
Formula: C17H14N2O
SMILES: Cc1ccc(NN=C2C(=O)C=Cc3ccccc32)cc1
Mol. weight [g/mol]: 262.31
CAS: 64022-28-2

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 157.47 | kJ/mol | Joback Method |
| hvap | 74.82 | kJ/mol | Joback Method |
| log10ws | -4.24 | | Crippen Method |
| logp | 3.407 | | Crippen Method |
| mcvol | 204.940 | ml/mol | McGowan Method |
| pc | 2324.78 | kPa | Joback Method |
| tb | 863.67 | K | Joback Method |
| tc | 1131.62 | K | Joback Method |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C64022282&Units=SI>
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>

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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