

Pulegone, 2,4-dinitrophenyl hydrazone

Inchi: InChI=1S/C16H20N4O4/c1-10(2)12-5-4-11(3)15(8-12)18-17-14-7-6-13(19(21)22)9-16(14)
InchiKey: WLFDFNUOQDTAZ-OBGWFSINSA-N
Formula: C16H20N4O4
SMILES: CC(C)=C1CCC(C)C(=NNc2ccc([N+](=O)[O-])cc2[N+](=O)[O-])C1
Mol. weight [g/mol]: 332.35

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 33.56 | kJ/mol | Joback Method |
| hvap | 99.87 | kJ/mol | Joback Method |
| log10ws | -6.21 | | Crippen Method |
| logp | 4.427 | | Crippen Method |
| mcvol | 247.880 | ml/mol | McGowan Method |
| pc | 1882.17 | kPa | Joback Method |
| tb | 1061.20 | K | Joback Method |
| tc | 1334.91 | K | Joback Method |

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=B6002097&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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