

3,4,5-Trimethoxyphenyl cyanate

Inchi: InChI=1S/C10H11NO4/c1-13-8-4-7(11-6-12)5-9(14-2)10(8)15-3/h4-5H,1-3H3
InchiKey: MJJXWPHZDBIHIM-UHFFFAOYSA-N
Formula: C10H11NO4
SMILES: COc1cc(N=C=O)cc(OC)c1OC
Mol. weight [g/mol]: 209.20
CAS: 1016-19-9

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -449.68 | kJ/mol | Joback Method |
| hvap | 58.88 | kJ/mol | Joback Method |
| log10ws | -6.31 | | Crippen Method |
| logp | 1.680 | | Crippen Method |
| mcvol | 152.860 | ml/mol | McGowan Method |
| pc | 2862.74 | kPa | Joback Method |
| tb | 603.75 | K | Joback Method |
| tc | 813.85 | K | Joback Method |

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1016199&Units=SI>

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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