

4-Isopropylphenyl isothiocyanate

Inchi: InChI=1S/C10H11NS/c1-8(2)9-3-5-10(6-4-9)11-7-12/h3-6,8H,1-2H3
InchiKey: SNWJJTIJIDXIHU-UHFFFAOYSA-N
Formula: C10H11NS
SMILES: CC(C)c1ccc(N=C=S)cc1
Mol. weight [g/mol]: 177.27
CAS: 89007-45-4

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 254.12 | kJ/mol | Joback Method |
| hvap | 50.84 | kJ/mol | Joback Method |
| log10ws | -3.57 | | Crippen Method |
| logp | 3.544 | | Crippen Method |
| mvol | 145.730 | ml/mol | McGowan Method |
| pc | 2979.54 | kPa | Joback Method |
| tb | 605.37 | K | Joback Method |
| tc | 860.42 | K | Joback Method |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C89007454&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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