

4-Fluoro-«alpha»-methylbenzyl isothiocyanate

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|----------------------|--|
| Inchi: | InChI=1S/C9H8FNS/c1-7(11-6-12)8-2-4-9(10)5-3-8/h2-5,7H,1H3 |
| InchiKey: | JXMBAXGHCKMDES-UHFFFAOYSA-N |
| Formula: | C9H8FNS |
| SMILES: | CC(N=C=S)c1ccc(F)cc1 |
| Mol. weight [g/mol]: | 181.23 |
| CAS: | 182565-27-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 78.65 | kJ/mol | Joback Method |
| hvap | 47.80 | kJ/mol | Joback Method |
| log10ws | -3.42 | | Crippen Method |
| logp | 2.990 | | Crippen Method |
| mcvol | 133.410 | ml/mol | McGowan Method |
| pc | 3152.62 | kPa | Joback Method |
| tb | 581.76 | K | Joback Method |
| tc | 829.25 | K | Joback Method |

Sources

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|-----------------|---|
| 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=C182565271&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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