# 4-Fluoro-«alpha»-methylbenzyl isothiocyanate

**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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C182565271&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**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 |