

Ketone, 5-methoxy-4-nitro-2-thienyl methyl

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|-----------------------------|--|
| Inchi: | InChI=1S/C7H7NO4S/c1-4(9)6-3-5(8(10)11)7(12-2)13-6/h3H,1-2H3 |
| InchiKey: | SYMXAAJYYZNWOY-UHFFFAOYSA-N |
| Formula: | C7H7NO4S |
| SMILES: | COc1sc(C(C)=O)cc1[N+](=O)[O-] |
| Mol. weight [g/mol]: | 201.20 |
| CAS: | 78150-61-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.66 | | Crippen Method |
| logp | 1.867 | | Crippen Method |
| mcvol | 131.240 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C78150615&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

Latest version available from:

<https://www.chemeo.com/cid/50-681-0/Ketone-5-methoxy-4-nitro-2-thienyl-methyl.pdf>

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