

Ketone, 5-acetamido-4-nitro-2-thienyl isobutyl

Inchi:	InChI=1S/C10H12N2O4S/c1-5(2)9(14)8-4-7(12(15)16)10(17-8)11-6(3)13/h4-5H,1-3H3,(H
InchiKey:	JSOMCJFFQRPXEM-UHFFFAOYSA-N
Formula:	C10H12N2O4S
SMILES:	CC(=O)Nc1sc(C(=O)C(C)C)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	256.28
CAS:	116373-99-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	2.453		Crippen Method
mcvol	179.190	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116373990&Units=SI

Legend

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

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