

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

Inchi:	InChI=1S/C8H10N2O3S/c1-4(2)7(11)6-3-5(10(12)13)8(9)14-6/h3-4H,9H2,1-2H3
InchiKey:	PDZNMUNHHSBCLG-UHFFFAOYSA-N
Formula:	C8H10N2O3S
SMILES:	CC(C)C(=O)c1cc([N+](=O)[O-])c(N)s1
Mol. weight [g/mol]:	214.24
CAS:	52499-06-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	2.077		Crippen Method
mcvol	149.440	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52499066&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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