

Ketone, 5-amino-4-nitro-2-thienyl-3,4-dichlorophenyl

Inchi: InChI=1S/C11H6Cl2N2O3S/c12-6-2-1-5(3-7(6)13)10(16)9-4-8(15(17)18)11(14)19-9/h1-4
InchiKey: VJLKOTCOOSHMG-P-UHFFFAOYSA-N
Formula: C11H6Cl2N2O3S
SMILES: Nc1sc(C(=O)c2ccc(Cl)c(Cl)c2)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 317.15
CAS: 99971-81-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	3.776		Crippen Method
mcvol	192.430	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C99971810&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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