

Acetophenone-«alpha»,«alpha»,«alpha»-d3

InChI: InChI=1S/C8H8O/c1-7(9)8-5-3-2-4-6-8/h2-6H,1H3/i1D3

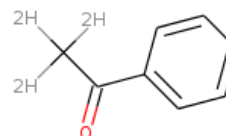
InChI Key: KWOLFJPFCHCOCG-FIBGUPNXSA-N

Formula: C8H5D3O

SMILES: [H]C([H])([H])C(=O)c1ccccc1

Molecular Weight: 123.17

CAS: 17537-31-4



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	1.889		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H8O/c1-7\(9\)8-5-3-2-4-6-8/h2-6H,1H3/i1D3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H8O/c1-7(9)8-5-3-2-4-6-8/h2-6H,1H3/i1D3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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