

2-Pyrrolidone carboxylic acid, N-trifluoroacetyl-, n-butyl ester

Other names: Pyroglutamic acid, butyl ester, TFA
Inchi: InChI=1S/C11H14F3NO4/c1-2-3-6-19-9(17)7-4-5-8(16)15(7)10(18)11(12,13)14/h7H,2-6H
InchiKey: ZEXNADZGHOHCRS-UHFFFAOYSA-N
Formula: C11H14F3NO4
SMILES: CCCCOC(=O)C1CCC(=O)N1C(=O)C(F)(F)F
Mol. weight [g/mol]: 281.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	1.410		Crippen Method
mcvol	180.860	ml/mol	McGowan Method
rinpol	1505.00		NIST Webbook
rinpol	1505.00		NIST Webbook

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=U328304&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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