

2-Butanone oxime, O-[(pentafluorophenyl)methyl]-

Other names: 2-Butanone, PFBO # 2
Inchi: InChI=1S/C11H10F5NO/c1-3-5(2)17-18-4-6-7(12)9(14)11(16)10(15)8(6)13/h3-4H2,1-2H3
InchiKey: LNDQFOSWZJYEIC-UHFFFAOYSA-N
Formula: C11H10F5NO
SMILES: CCC(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 267.20

Physical Properties

Property code	Value	Unit	Source
logp	3.685		Crippen Method
mcvol	162.490	ml/mol	McGowan Method
ripol	1521.00		NIST Webbook
ripol	1521.00		NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U288170&Units=SI>

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-472-3/2-Butanone-oxime-O-pentafluorophenyl-methyl.pdf>

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