n-Undecanal, O-[(pentafluorophenyl)methyl]oxime

Other names: Undecanal, PFBO # 2
Inchi: InChI=1S/C18H24F5NO/c1-2-3-4-5-6-7-8-9-10-11-24-25-12-13-14(19)16(21)18(23)17(22
InchiKey: XJDXRHQPJGTNHN-UHFFFAOYSA-N
Formula: C18H24F5NO
SMILES: CCCCCCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 365.39

Physical Properties

Property code	Value	Unit	Source
logp	6.415		Crippen Method
mcvol	261.120	ml/mol	McGowan Method
ripol	2243.00		NIST Webbook
ripol	2243.00		NIST Webbook
tb	570.20	K	Cheméo Relay (1.0)

Sources

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=U288102&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices
tb: Normal Boiling Point Temperature