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

Other names: Octanal, O-[(pentafluorophenyl)methyl]oxime, (E)
Octanal, PFBO # 2

Inchi: InChI=1S/C15H18F5NO/c1-2-3-4-5-6-7-8-21-22-9-10-11(16)13(18)15(20)14(19)12(10)17

InchiKey: RLSQIXNUITTXKZ-UHFFFAOYSA-N

Formula: C15H18F5NO

SMILES: CCCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 323.30

Physical Properties

Property code	Value	Unit	Source
logp	5.245		Crippen Method
mcvol	218.850	ml/mol	McGowan Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1950.00		NIST Webbook
tb	534.18	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U288097&Units=SI

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

Legend

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature