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

Other names: Heptanal, PFBO # 2
Inchi: InChI=1S/C14H16F5NO/c1-2-3-4-5-6-7-20-21-8-9-10(15)12(17)14(19)13(18)11(9)16/h7H
InchiKey: OZZBQOMRSSEYJF-UHFFFAOYSA-N
Formula: C14H16F5NO
SMILES: CCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 309.28

Physical Properties

Property code	Value	Unit	Source
logp	4.855		Crippen Method
mcvol	204.760	ml/mol	McGowan Method
rinpol	1558.00		NIST Webbook
rinpol	1558.00		NIST Webbook
ripol	1861.00		NIST Webbook
tb	521.22	K	Cheméo Relay (1.0)

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=U288096&Units=SI

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