6-Methyl-5-hepten-2-one oxime, o-[(pentafluorophenyl)methyl]-

Other names: 6-Methyl-5-hepten-2-one, PFBO # 2
Inchi: InChI=1S/C15H16F5NO/c1-8(2)5-4-6-9(3)21-22-7-10-11(16)13(18)15(20)14(19)12(10)17
InchiKey: UNYXAVQWMIOYNJ-UHFFFAOYSA-N
Formula: C15H16F5NO
SMILES: CC(C)=CCCC(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 321.29

Physical Properties

Property code	Value	Unit	Source
hf	-1106.66	kJ/mol	Joback Method
hvap	56.33	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.021		Crippen Method
mcvol	214.550	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
ripol	1883.00		NIST Webbook
ripol	1883.00		NIST Webbook
tb	693.55	K	Joback Method
tc	877.87	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U288124&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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