n-Hexanal, o-[(pentafluorophenyl)methyl]oxime

Other names: Hexanal, PFBO, # 2

Inchi: InChI=1S/C13H14F5NO/c1-2-3-4-5-6-19-20-7-8-9(14)11(16)13(18)12(17)10(8)15/h6H,2-

InchiKey: GPAVMFOMYSGJDM-UHFFFAOYSA-N

Formula: C13H14F5NO

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

Mol. weight [g/mol]: 295.25

Physical Properties

Property code	Value	Unit	Source
hf	-1163.02	kJ/mol	Joback Method
hvap	51.76	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.465		Crippen Method
mcvol	190.670	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1765.00		NIST Webbook
tb	643.87	K	Joback Method
tc	819.87	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U288098&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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