trans-2-Hexenal oxime, o-[(pentafluorophenyl)methyl]-

Other names: (E)-2-Hexenal, PFBO # 2
Inchi: InChI=1S/C13H12F5NO/c1-2-3-4-5-6-19-20-7-8-9(14)11(16)13(18)12(17)10(8)15/h4-6H,
InchiKey: UFLHMANGSVRSPF-VVILYHCASA-N
Formula: C13H12F5NO
SMILES: CCCC=CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 293.23

Physical Properties

Property code	Value	Unit	Source
hf	-1045.80	kJ/mol	Joback Method
hvap	51.72	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.241		Crippen Method
mcvol	186.370	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
rinpol	1522.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1910.00		NIST Webbook
tb	648.03	K	Joback Method
tc	829.81	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=U288149&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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