Propenal O-pentafluorophenylmethyl-oxime

Other names:	Acrolein O-2,3,4,5,6-PFBHA-oxime
	2-Propenal, PFBO # 2
Inchi:	InChI=1S/C10H6F5NO/c1-2-3-16-17-4-5-6(11)8(13)10(15)9(14)7(5)12/h2-3H,1,4H2
InchiKey:	ICDUEGOPUWNJNF-UHFFFAOYSA-N
Formula:	C10H6F5NO
SMILES:	C=CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	251.15

Physical Properties

Property code	Value	Unit	Source
hf	-975.67	kJ/mol	Joback Method
hvap	44.41	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.071		Crippen Method
mcvol	144.100	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1201.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1594.00		NIST Webbook
tb	571.91	K	Joback Method
tc	754.69	K	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372214&Units=SI

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