2-Propenal, PFBO # 1

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	1186.00		NIST Webbook
rinpol	1186.00		NIST Webbook
ripol	1566.00		NIST Webbook
tb	571.91	K	Joback Method
tc	754.69	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=R574859&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