Ethanal, PFBO # 1

Inchi: InChI=1S/C9H6F5NO/c1-2-15-16-3-4-5(10)7(12)9(14)8(13)6(4)11/h2H,3H2,1H3
InchiKey: AKDRYEADQPNLOH-UHFFFAOYSA-N
Formula: C9H6F5NO
SMILES: CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 239.14

Physical Properties

Property code	Value	Unit	Source
hf	-1080.46	kJ/mol	Joback Method
hvap	42.85	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	2.904		Crippen Method
mcvol	134.310	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1104.00		NIST Webbook
rinpol	1104.00		NIST Webbook
ripol	1451.00		NIST Webbook
tb	552.35	K	Joback Method
tc	733.73	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=R575703&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