Cinnamic aldehyde, PFBO # 2

Inchi: InChI=1S/C16H10F5NO/c17-12-11(13(18)15(20)16(21)14(12)19)9-23-22-8-4-7-10-5-2-1-
InchiKey: LIDMFHBBTNZNCB-YEQYMXEUSA-N
Formula: C16H10F5NO
SMILES: Fc1c(F)c(F)c(CON=CC=Cc2ccccc2)c(F)c1F
Mol. weight [g/mol]: 327.25

Physical Properties

Property code	Value	Unit	Source
hf	-871.19	kJ/mol	Joback Method
hvap	60.67	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	4.598		Crippen Method
mcvol	204.880	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	1993.00		NIST Webbook
ripol	2759.00		NIST Webbook
tb	743.35	K	Joback Method
tc	950.32	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=R575332&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