Benzaldehyde, PFBO # 1

Inchi: InChI=1S/C14H8F5NO/c15-10-9(11(16)13(18)14(19)12(10)17)7-21-20-6-8-4-2-1-3-5-8/h
InchiKey: UKSAZCDAGVHMRF-UHFFFAOYSA-N
Formula: C14H8F5NO
SMILES: Fc1c(F)c(F)c(CON=Cc2ccccc2)c(F)c1F
Mol. weight [g/mol]: 301.21

Physical Properties

Property code	Value	Unit	Source
hf	-947.13	kJ/mol	Joback Method
hvap	56.26	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.933		Crippen Method
mcvol	181.000	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1667.00		NIST Webbook
tb	693.43	K	Joback Method
tc	898.29	K	Joback Method

Sources

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=R575243&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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