4-Hydroxy-3-methoxybenzaldehyde, PFBO # 1

Inchi: InChI=1S/C15H10F5NO3/c1-23-10-4-7(2-3-9(10)22)5-21-24-6-8-11(16)13(18)15(20)14(1

InchiKey: SUAYPXFACRNFGO-UHFFFAOYSA-N

Formula: C15H10F5NO3

SMILES: COc1cc(C=NOCc2c(F)c(F)c(F)c(F)c2F)ccc1O

Mol. weight [g/mol]: 347.24

Physical Properties

Property code	Value	Unit	Source
hf	-1288.77	kJ/mol	Joback Method
hvap	74.57	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.647		Crippen Method
mcvol	206.830	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2060.00		NIST Webbook
ripol	3140.00		NIST Webbook
tb	824.33	K	Joback Method
tc	1035.76	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575010&Units=SI

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

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