4-Hydroxy-3,5-dimethoxybenzaldehyde, PFBO # 1

Inchi: InChI=1S/C16H12F5NO4/c1-24-9-3-7(4-10(25-2)16(9)23)5-22-26-6-8-11(17)13(19)15(21
InchiKey: VWHYOHDIHCDNMH-UHFFFAOYSA-N
Formula: C16H12F5NO4
SMILES: COc1cc(C=NOCc2c(F)c(F)c(F)c(F)c2F)cc(OC)c1O
Mol. weight [g/mol]: 377.26

Physical Properties

Property code	Value	Unit	Source
hf	-1453.10	kJ/mol	Joback Method
hvap	79.87	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	3.656		Crippen Method
mcvol	226.790	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	874.61	K	Joback Method
tc	1086.19	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R576048&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature