Acetophenone, 4'-hydroxy-3'-methoxy, PFBO # 1

Inchi: InChI=1S/C16H12F5NO3/c1-7(8-3-4-10(23)11(5-8)24-2)22-25-6-9-12(17)14(19)16(21)15(20)13(9)18/ccc1O

InchiKey: LHUFENWHXCIVAC-UHFFFAOYSA-N

Formula: C16H12F5NO3

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

Mol. weight [g/mol]: 361.26

Physical Properties

Property code	Value	Unit	Source
hf	-1319.20	kJ/mol	Joback Method
hvap	76.88	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.037		Crippen Method
mcvol	220.920	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2037.00		NIST Webbook
ripol	3176.00		NIST Webbook
tb	847.09	K	Joback Method
tc	1059.61	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=R575189&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