Acetophenone, 4'-methoxy, PFBO # 1

Inchi: InChI=1S/C16H12F5NO2/c1-8(9-3-5-10(23-2)6-4-9)22-24-7-11-12(17)14(19)16(21)15(20

InchiKey: NSIBFOZGYKUYQJ-UHFFFAOYSA-N

Formula: C16H12F5NO2

SMILES: COc1ccc(C(C)=NOCc2c(F)c(F)c(F)c(F)c2F)cc1

Mol. weight [g/mol]: 345.26

Physical Properties

Property code	Value	Unit	Source
hf	-1141.89	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.332		Crippen Method
mcvol	215.050	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	1906.00		NIST Webbook
ripol	2613.00		NIST Webbook
tb	766.47	K	Joback Method
tc	969.49	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=R575203&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