Acetophenone, 3',5'-dimethyl, PFBO # 1

Inchi: InChI=1S/C17H14F5NO/c1-8-4-9(2)6-11(5-8)10(3)23-24-7-12-13(18)15(20)17(22)16(21)
InchiKey: XYRDULNMMSQCON-UHFFFAOYSA-N
Formula: C17H14F5NO
SMILES: CC(=NOCc1c(F)c(F)c(F)c(F)c1F)c1cc(C)cc(C)c1
Mol. weight [g/mol]: 343.29

Physical Properties

Property code	Value	Unit	Source
hf	-1041.78	kJ/mol	Joback Method
hvap	64.34	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	4.940		Crippen Method
mcvol	223.270	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
ripol	2227.00		NIST Webbook
tb	771.91	K	Joback Method
tc	975.02	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575169&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature