2-Butanone, 4-phenyl, PFBO # 2

Inchi: InChI=1S/C17H14F5NO/c1-10(7-8-11-5-3-2-4-6-11)23-24-9-12-13(18)15(20)17(22)16(21
InchiKey: GMYACCNXCMIGHE-UHFFFAOYSA-N
Formula: C17H14F5NO
SMILES: CC(CCc1ccccc1)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 343.29

Physical Properties

Property code	Value	Unit	Source
hf	-1018.84	kJ/mol	Joback Method
hvap	63.02	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	4.907		Crippen Method
mcvol	223.270	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	2148.00		NIST Webbook
tb	761.95	K	Joback Method
tc	963.45	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R574720&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