Acetophenone, PFBO # 2

Inchi: InChI=1S/C15H10F5NO/c1-8(9-5-3-2-4-6-9)21-22-7-10-11(16)13(18)15(20)14(19)12(10)
InchiKey: MICGAUDRWWJXQO-UHFFFAOYSA-N
Formula: C15H10F5NO
SMILES: CC(=NOCc1c(F)c(F)c(F)c(F)c1F)c1ccccc1
Mol. weight [g/mol]: 315.24

Physical Properties

Property code	Value	Unit	Source
hf	-977.56	kJ/mol	Joback Method
hvap	58.57	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.323		Crippen Method
mcvol	195.090	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	1739.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2295.00		NIST Webbook
tb	716.19	K	Joback Method
tc	921.45	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575238&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

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

Latest version available from:
https://www.chemeo.com/cid/60-866-4/Acetophenone-PFBO-2.pdf
Generated by Cheméo on 2024-04-18 06:29:57.092177854 +0000 UTC m=+15711046.012755165.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.