2-Methyl-3-heptanone, PFBO # 1

Inchi: InChI=1S/C15H18F5NO/c1-4-5-6-10(8(2)3)21-22-7-9-11(16)13(18)15(20)14(19)12(9)17/
InchiKey: MVHPLUGMPFYDEJ-UHFFFAOYSA-N
Formula: C15H18F5NO
SMILES: CCCCC(=NOCc1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]: 323.30

Physical Properties

Property code	Value	Unit	Source
hf	-1219.37	kJ/mol	Joback Method
hvap	55.90	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.101		Crippen Method
mcvol	218.850	ml/mol	McGowan Method
pc	1335.88	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
ripol	1671.00		NIST Webbook
tb	689.07	K	Joback Method
tc	868.47	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R574755&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