6-Methyl-3,5-heptadien-2-one, PFBO # 2

Inchi: InChI=1S/C15H14F5NO/c1-8(2)5-4-6-9(3)21-22-7-10-11(16)13(18)15(20)14(19)12(10)17

InchiKey: FMXNZZXBMGGAHJ-GHFMCXKOSA-N

Formula: C15H14F5NO

SMILES: CC(C)=CC=CC(C)=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 319.27

Physical Properties

Property code	Value	Unit	Source
hf	-989.44	kJ/mol	Joback Method
hvap	56.28	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.797		Crippen Method
mcvol	210.250	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	1756.00		NIST Webbook
tb	697.71	K	Joback Method
tc	887.70	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575085&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

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