3-Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl), PFBO # 2

Inchi: InChI=1S/C20H22F5NO/c1-11-6-5-9-20(3,4)14(11)8-7-12(2)26-27-10-13-15(21)17(23)19

InchiKey: FVBURQNDSXBUAV-SRGMPAQCSA-N

Formula: C20H22F5NO

SMILES: CC1=CCCC(C)(C)C1C=CC(C)=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 387.39

Physical Properties

Property code	Value	Unit	Source
hf	-1104.54	kJ/mol	Joback Method
hvap	67.30	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	6.213		Crippen Method
mcvol	269.840	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
ripol	2400.00		NIST Webbook
tb	827.33	K	Joback Method
tc	1033.35	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R574908&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