4-Oxo-2-nonenal, bis-PFBO, # 1

Inchi: InChI=1S/C23H18F10N2O2/c1-2-3-4-6-11(35-37-10-13-16(26)20(30)23(33)21(31)17(13)
InchiKey: ADKWDTVFGFCPNR-UTTZIMMKSA-N
Formula: C23H18F10N2O2
SMILES: CCCCCC(C=CC=NOCc1c(F)c(F)c(F)c(F)c1F)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 544.39

Physical Properties

Property code	Value	Unit	Source
hf	-2113.36	kJ/mol	Joback Method
hvap	81.28	kJ/mol	Joback Method
log10ws	-10.30		Crippen Method
logp	7.289		Crippen Method
mcvol	323.910	ml/mol	McGowan Method
pc	793.05	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	1023.74	K	Joback Method
tc	1259.39	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R398917&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