Diacetyl, PFBO # 1

Inchi: InChI=1S/C18H10F10N2O2/c1-5(29-31-3-7-9(19)13(23)17(27)14(24)10(7)20)6(2)30-32-4
InchiKey: FJVTVBQIHZZDBE-UHFFFAOYSA-N
Formula: C18H10F10N2O2
SMILES: CC(=NOCc1c(F)c(F)c(F)c(F)c1F)C(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 476.27

Physical Properties

Property code	Value	Unit	Source
hf	-2137.17	kJ/mol	Joback Method
hvap	70.27	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	5.563		Crippen Method
mcvol	257.760	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	1319.00		NIST Webbook
rinpol	1319.00		NIST Webbook
ripol	1761.00		NIST Webbook
tb	905.06	K	Joback Method
tc	1108.96	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575367&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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