Nitrobenzene, 3-trifluoroacetylamino-4-trifluoroacetyloxy-

Inchi: InChI=1S/C10H4F6N2O5/c11-9(12,13)7(19)17-5-3-4(18(21)22)1-2-6(5)23-8(20)10(14,15

InchiKey: FDSRBYSCQBQBBA-UHFFFAOYSA-N

Formula: C10H4F6N2O5

SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1N=C(O)C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 346.14

Physical Properties

Property code	Value	Unit	Source
hf	-1565.66	kJ/mol	Joback Method
hvap	79.78	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.213		Crippen Method
mcvol	175.030	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	850.87	K	Joback Method
tc	1062.09	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374265&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

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