Benzamide, N-(3-nitrophenyl)-2,6-difluoro-

Inchi: InChI=1S/C13H8F2N2O3/c14-10-5-2-6-11(15)12(10)13(18)16-8-3-1-4-9(7-8)17(19)20/h1
InchiKey: QCVSMYWOKQQNCW-UHFFFAOYSA-N
Formula: C13H8F2N2O3
SMILES: O=[N+]([O-])c1cccc(N=C(O)c2c(F)cccc2F)c1
Mol. weight [g/mol]: 278.21
CAS: 294852-79-2

Physical Properties

Property code	Value	Unit	Source
hf	-355.78	kJ/mol	Joback Method
hvap	86.10	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.509		Crippen Method
mcvol	179.020	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	884.26	K	Joback Method
tc	1125.46	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C294852792&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