Benzamide, N-(2-iodo-4-methylphenyl)-2,3,4-trifluoro-

Inchi: InChI=1S/C14H9F3INO/c1-7-2-5-11(10(18)6-7)19-14(20)8-3-4-9(15)13(17)12(8)16/h2-6H

InchiKey: GBSGBFFGEVDUGF-UHFFFAOYSA-N

Formula: C14H9F3INO

SMILES: Cc1ccc(N=C(O)c2ccc(F)c(F)c2F)c(I)c1

Mol. weight [g/mol]: 391.13

Physical Properties

Property code	Value	Unit	Source
hf	-507.84	kJ/mol	Joback Method
hvap	81.61	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.653		Crippen Method
mcvol	203.280	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	857.67	K	Joback Method
tc	1091.37	K	Joback Method

Sources

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=U307181&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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