trans-Cinnamamide, N-(2-iodo-4-methylphenyl)-3-trifluoromethyl-

Inchi: InChI=1S/C17H13F3INO/c1-11-5-7-15(14(21)9-11)22-16(23)8-6-12-3-2-4-13(10-12)17(18

InchiKey: ICFOMNUAVOZDPE-SOFGYWHQSA-N

Formula: C17H13F3INO

SMILES: Cc1ccc(N=C(O)C=Cc2cccc(C(F)(F)F)c2)c(I)c1

Mol. weight [g/mol]: 431.19

Physical Properties

Property code	Value	Unit	Source
hf	-438.35	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.920		Crippen Method
mcvol	241.250	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	2700.00		NIST Webbook
rinpol	2700.00		NIST Webbook
tb	917.28	K	Joback Method
tc	1157.31	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307372&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