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

Inchi: InChI=1S/C15H14INO/c1-10-4-3-5-12(8-10)15(18)17-14-7-6-11(2)9-13(14)16/h3-9H,1-2H

InchiKey: LRRRGSNFNASUFB-UHFFFAOYSA-N

Formula: C15H14INO

SMILES: Cc1cccc(C(O)=Nc2ccc(C)cc2I)c1

Mol. weight [g/mol]: 351.18

Physical Properties

Property code	Value	Unit	Source
hf	82.79	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.544		Crippen Method
mcvol	212.060	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	2556.00		NIST Webbook
rinpol	2556.00		NIST Webbook
tb	872.78	K	Joback Method
tc	1127.87	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307119&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