

Acetamide, N-(2-iodo-4-methylphenyl)-2-phenyl-

Inchi:	InChI=1S/C15H14INO/c1-11-7-8-14(13(16)9-11)17-15(18)10-12-5-3-2-4-6-12/h2-9H,10H
InchiKey:	ZPQAQSTUVKQDFQ-UHFFFAOYSA-N
Formula:	C15H14INO
SMILES:	Cc1ccc(N=C(O)Cc2ccccc2)c(I)c1
Mol. weight [g/mol]:	351.18

Physical Properties

Property code	Value	Unit	Source
hf	94.26	kJ/mol	Joback Method
hvap	84.31	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.430		Crippen Method
mcvol	212.060	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	2474.00		NIST Webbook
rinpol	2474.00		NIST Webbook
tb	867.80	K	Joback Method
tc	1122.21	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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