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

Inchi: InChI=1S/C15H14INO2/c1-10-6-7-14(13(16)8-10)17-15(18)11-4-3-5-12(9-11)19-2/h3-9H

InchiKey: LVEFVYSATMNZOR-UHFFFAOYSA-N

Formula: C15H14INO2

SMILES: COc1cccc(C(=O)Nc2ccc(C)cc2I)c1

Mol. weight [g/mol]: 367.18

Physical Properties

Property code	Value	Unit	Source
gf	184.94	kJ/mol	Joback Method
hf	-28.74	kJ/mol	Joback Method
hfus	33.81	kJ/mol	Joback Method
hvap	80.49	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.861		Crippen Method
mcvol	217.930	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tb	830.50	K	Joback Method
tc	1090.02	K	Joback Method
tf	532.09	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.59	J/mol×K	830.50	Joback Method
cpg	570.96	J/mol×K	873.75	Joback Method
cpg	582.16	J/mol×K	917.01	Joback Method
cpg	592.25	J/mol×K	960.26	Joback Method
cpg	601.30	J/mol×K	1003.52	Joback Method
cpg	609.37	J/mol×K	1046.77	Joback Method
cpg	616.52	J/mol×K	1090.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306974&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume