

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

Inchi:	InChI=1S/C15H14INO2/c1-10-3-8-14(13(16)9-10)17-15(18)11-4-6-12(19-2)7-5-11/h3-9H
InchiKey:	MIULEBGUUCEXPI-UHFFFAOYSA-N
Formula:	C15H14INO2
SMILES:	COc1ccc(C(=O)Nc2ccc(C)cc2I)cc1
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
rinsol	2753.00		NIST Webbook
tb	830.50	K	Joback Method
tc	1090.02	K	Joback Method
tf	532.09	K	Joback Method
vc	0.806	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307501&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

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

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