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

Inchi: InChI=1S/C14H11ClINO/c1-9-6-7-13(12(16)8-9)17-14(18)10-4-2-3-5-11(10)15/h2-8H,1H
InchiKey: IOADKGPOYDBUMD-UHFFFAOYSA-N
Formula: C14H11ClINO
SMILES: Cc1ccc(NC(=O)c2ccccc2Cl)c(I)c1
Mol. weight [g/mol]: 371.60

Physical Properties

Property code	Value	Unit	Source
gf	269.59	kJ/mol	Joback Method
hf	108.38	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	80.24	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.505		Crippen Method
mcvol	210.210	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	822.63	K	Joback Method
tc	1094.02	K	Joback Method
tf	528.51	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.71	J/mol×K	822.63	Joback Method
cpg	511.86	J/mol×K	867.86	Joback Method
cpg	521.96	J/mol×K	913.09	Joback Method
cpg	531.11	J/mol×K	958.32	Joback Method
cpg	539.40	J/mol×K	1003.56	Joback Method
cpg	546.96	J/mol×K	1048.79	Joback Method
cpg	553.86	J/mol×K	1094.02	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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