2-Iodo-N-phenylbenzamide

Inchi: InChI=1S/C13H10INO/c14-12-9-5-4-8-11(12)13(16)15-10-6-2-1-3-7-10/h1-9H,(H,15,16)
InchiKey: LJOZMWRYMKECFF-UHFFFAOYSA-N
Formula: C13H10INO
SMILES: O=C(Nc1ccccc1)c1ccccc1I
Mol. weight [g/mol]: 323.13

Physical Properties

Property code	Value	Unit	Source
gf	292.36	kJ/mol	Joback Method
hf	167.70	kJ/mol	Joback Method
hfus	28.22	kJ/mol	Joback Method
hvap	72.30	kJ/mol	Joback Method
log10ws	-4.21		Aqueous Solubility Prediction Method
logp	3.543		Crippen Method
mcvol	183.880	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	752.36	K	Joback Method
tc	1028.05	K	Joback Method
tf	462.28	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.17	J/mol×K	752.36	Joback Method
cpg	444.31	J/mol×K	798.31	Joback Method
cpg	455.24	J/mol×K	844.26	Joback Method
cpg	465.10	J/mol×K	890.20	Joback Method
cpg	474.00	J/mol×K	936.15	Joback Method
cpg	482.06	J/mol×K	982.10	Joback Method
cpg	489.41	J/mol×K	1028.05	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume