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

Inchi: InChI=1S/C14H11BrINO/c1-9-5-6-13(12(16)7-9)17-14(18)10-3-2-4-11(15)8-10/h2-8H,1H

InchiKey: VQNZCBSMPFSSTN-UHFFFAOYSA-N

Formula: C14H11BrINO

SMILES: Cc1ccc(NC(=O)c2cccc(Br)c2)c(I)c1

Mol. weight [g/mol]: 416.05

Physical Properties

Property code	Value	Unit	Source
gf	295.84	kJ/mol	Joback Method
hf	150.45	kJ/mol	Joback Method
hfus	35.32	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.614		Crippen Method
mcvol	215.470	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	2732.00		NIST Webbook
rinpol	2732.00		NIST Webbook
tb	851.36	K	Joback Method
tc	1130.09	K	Joback Method
tf	558.39	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.48	J/mol×K	851.36	Joback Method
cpg	519.21	J/mol×K	897.82	Joback Method
cpg	528.97	J/mol×K	944.27	Joback Method
cpg	537.89	J/mol×K	990.73	Joback Method
cpg	546.09	J/mol×K	1037.18	Joback Method
cpg	553.71	J/mol×K	1083.64	Joback Method
cpg	560.85	J/mol×K	1130.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307159&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

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