Butanamide, N-(2-iodo-4-methylphenyl)-

Inchi: InChI=1S/C11H14INO/c1-3-4-11(14)13-10-6-5-8(2)7-9(10)12/h5-7H,3-4H2,1-2H3,(H,13,1
InchiKey: IBNLKTMCQORLLV-UHFFFAOYSA-N
Formula: C11H14INO
SMILES: CCCC(=O)Nc1ccc(C)cc1I
Mol. weight [g/mol]: 303.14

Physical Properties

Property code	Value	Unit	Source
gf	153.48	kJ/mol	Joback Method
hf	-39.02	kJ/mol	Joback Method
hfus	28.61	kJ/mol	Joback Method
hvap	66.23	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.338		Crippen Method
mcvol	179.460	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1978.00		NIST Webbook
tb	684.90	K	Joback Method
tc	923.86	K	Joback Method
tf	425.84	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.40	J/mol×K	684.90	Joback Method
cpg	431.16	J/mol×K	724.73	Joback Method
cpg	443.00	J/mol×K	764.55	Joback Method
cpg	453.99	J/mol×K	804.38	Joback Method
cpg	464.18	J/mol×K	844.21	Joback Method
cpg	473.62	J/mol×K	884.03	Joback Method
cpg	482.35	J/mol×K	923.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306919&Units=SI

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