Propanamide, N-(2-iodo-4-methylphenyl)-3-chloro-

Inchi: InChI=1S/C10H11ClINO/c1-7-2-3-9(8(12)6-7)13-10(14)4-5-11/h2-3,6H,4-5H2,1H3,(H,13,

InchiKey: CRLIKQMWVMLNQX-UHFFFAOYSA-N

Formula: C10H11ClINO

SMILES: Cc1ccc(NC(=O)CCCl)c(I)c1

Mol. weight [g/mol]: 323.56

Physical Properties

Property code	Value	Unit	Source
gf	133.13	kJ/mol	Joback Method
hf	-34.12	kJ/mol	Joback Method
hfus	30.22	kJ/mol	Joback Method
hvap	68.39	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.167		Crippen Method
mcvol	177.610	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	2137.00		NIST Webbook
rinpol	2137.00		NIST Webbook
tb	699.45	K	Joback Method
tc	946.03	K	Joback Method
tf	444.49	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.91	J/mol×K	699.45	Joback Method
cpg	401.90	J/mol×K	740.55	Joback Method
cpg	412.05	J/mol×K	781.64	Joback Method
cpg	421.40	J/mol×K	822.74	Joback Method
cpg	430.01	J/mol×K	863.83	Joback Method
cpg	437.95	J/mol×K	904.93	Joback Method
cpg	445.25	J/mol×K	946.03	Joback Method

Sources

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=U307231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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