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

Inchi: InChI=1S/C9H9ClINO/c1-6-2-3-8(7(11)4-6)12-9(13)5-10/h2-4H,5H2,1H3,(H,12,13)
InchiKey: LFRNCVLQAZNXIS-UHFFFAOYSA-N
Formula: C9H9ClINO
SMILES: Cc1ccc(NC(=O)CCl)c(I)c1
Mol. weight [g/mol]: 309.53

Physical Properties

Property code	Value	Unit	Source
gf	124.71	kJ/mol	Joback Method
hf	-13.48	kJ/mol	Joback Method
hfus	27.63	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.777		Crippen Method
mcvol	163.520	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1920.00		NIST Webbook
tb	676.57	K	Joback Method
tc	928.74	K	Joback Method
tf	433.22	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.25	J/mol×K	676.57	Joback Method
cpg	352.46	J/mol×K	718.60	Joback Method
cpg	361.85	J/mol×K	760.63	Joback Method
cpg	370.48	J/mol×K	802.66	Joback Method
cpg	378.40	J/mol×K	844.69	Joback Method
cpg	385.66	J/mol×K	886.72	Joback Method
cpg	392.32	J/mol×K	928.74	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=U307242&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