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

Inchi: InChI=1S/C10H11ClINO/c1-6-3-4-9(8(12)5-6)13-10(14)7(2)11/h3-5,7H,1-2H3,(H,13,14)
InchiKey: ZEFWFZBQZSRJBP-UHFFFAOYSA-N
Formula: C10H11ClINO
SMILES: Cc1ccc(NC(=O)C(C)Cl)c(I)c1
Mol. weight [g/mol]: 323.56

Physical Properties

Property code	Value	Unit	Source
gf	130.69	kJ/mol	Joback Method
hf	-39.40	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	68.01	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.165		Crippen Method
mcvol	177.610	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1936.00		NIST Webbook
rinpol	1936.00		NIST Webbook
tb	699.01	K	Joback Method
tc	950.73	K	Joback Method
tf	429.49	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.51	J/mol×K	699.01	Joback Method
cpg	402.75	J/mol×K	740.96	Joback Method
cpg	413.10	J/mol×K	782.92	Joback Method
cpg	422.61	J/mol×K	824.87	Joback Method
cpg	431.33	J/mol×K	866.82	Joback Method
cpg	439.33	J/mol×K	908.77	Joback Method
cpg	446.67	J/mol×K	950.73	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=U307490&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

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