Pentanamide, N-(2-iodo-4-methylphenyl)-5-chloro-

Inchi: InChI=1S/C12H15ClINO/c1-9-5-6-11(10(14)8-9)15-12(16)4-2-3-7-13/h5-6,8H,2-4,7H2,1H

InchiKey: FJWHSFDVCRTPGH-UHFFFAOYSA-N

Formula: C12H15ClINO

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

Mol. weight [g/mol]: 351.61

Physical Properties

Property code	Value	Unit	Source
gf	149.97	kJ/mol	Joback Method
hf	-75.40	kJ/mol	Joback Method
hfus	35.40	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.947		Crippen Method
mcvol	205.790	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	2382.00		NIST Webbook
tb	745.21	K	Joback Method
tc	981.88	K	Joback Method
tf	467.03	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.30	J/mol×K	745.21	Joback Method
cpg	504.54	J/mol×K	784.65	Joback Method
cpg	515.89	J/mol×K	824.10	Joback Method
cpg	526.40	J/mol×K	863.54	Joback Method
cpg	536.14	J/mol×K	902.99	Joback Method
cpg	545.17	J/mol×K	942.43	Joback Method
cpg	553.53	J/mol×K	981.88	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=U307364&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