Isopropyl-o-chlorocarbanilate

Inchi: InChI=1S/C10H12ClNO2/c1-7(2)14-10(13)12-9-6-4-3-5-8(9)11/h3-7H,1-2H3,(H,12,13)
InchiKey: YLZUJFLALUCJQI-UHFFFAOYSA-N
Formula: C10H12ClNO2
SMILES: CC(C)OC(=O)Nc1ccccc1Cl
Mol. weight [g/mol]: 213.66
CAS: 2150-22-3

Physical Properties

Property code	Value	Unit	Source
gf	-22.80	kJ/mol	Joback Method
hf	-237.02	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	60.38	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.297		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
tb	623.31	K	Joback Method
tc	845.22	K	Joback Method
tf	381.14	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.44	J/mol×K	623.31	Joback Method
cpg	386.15	J/mol×K	660.30	Joback Method
cpg	398.05	J/mol×K	697.28	Joback Method
cpg	409.13	J/mol×K	734.27	Joback Method
cpg	419.44	J/mol×K	771.25	Joback Method
cpg	428.97	J/mol×K	808.24	Joback Method
cpg	437.76	J/mol×K	845.22	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=C2150223&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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