5'-Chloro-2'-methoxy-2-methylvaleranilide

Inchi: InChI=1S/C13H18ClNO2/c1-4-5-9(2)13(16)15-11-8-10(14)6-7-12(11)17-3/h6-9H,4-5H2,1
InchiKey: YFWAXWYCHZLBET-UHFFFAOYSA-N
Formula: C13H18ClNO2
SMILES: CCCC(C)C(=O)Nc1cc(Cl)ccc1OC
Mol. weight [g/mol]: 255.74
CAS: 209683-34-1

Physical Properties

Property code	Value	Unit	Source
gf	-7.17	kJ/mol	Joback Method
hf	-310.41	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	67.72	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.723		Crippen Method
mcvol	199.930	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
tb	696.93	K	Joback Method
tc	908.92	K	Joback Method
tf	427.47	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.63	J/mol×K	696.93	Joback Method
cpg	537.94	J/mol×K	732.26	Joback Method
cpg	551.36	J/mol×K	767.59	Joback Method
cpg	563.90	J/mol×K	802.93	Joback Method
cpg	575.57	J/mol×K	838.26	Joback Method
cpg	586.41	J/mol×K	873.59	Joback Method
cpg	596.43	J/mol×K	908.92	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=C209683341&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