3'-chloro,4'-methylpropioanilide

Inchi: InChI=1S/C10H12ClNO/c1-3-10(13)12-8-5-4-7(2)9(11)6-8/h4-6H,3H2,1-2H3,(H,12,13)
InchiKey: DJKZTHGBRJVGNO-UHFFFAOYSA-N
Formula: C10H12ClNO
SMILES: CCC(=O)Nc1ccc(C)c(Cl)c1
Mol. weight [g/mol]: 197.66

Physical Properties

Property code	Value	Unit	Source
gf	75.01	kJ/mol	Joback Method
hf	-110.99	kJ/mol	Joback Method
hfus	25.81	kJ/mol	Joback Method
hvap	59.02	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.997		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	1736.00		NIST Webbook
tb	606.31	K	Joback Method
tc	827.43	K	Joback Method
tf	386.43	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.25	J/mol×K	606.31	Joback Method
cpg	360.66	J/mol×K	643.16	Joback Method
cpg	372.29	J/mol×K	680.02	Joback Method
cpg	383.17	J/mol×K	716.87	Joback Method
cpg	393.33	J/mol×K	753.72	Joback Method
cpg	402.80	J/mol×K	790.58	Joback Method
cpg	411.60	J/mol×K	827.43	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=R149156&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume