3'-chloro,4'-methylcaproanilide

Inchi: InChI=1S/C13H18ClNO/c1-3-4-5-6-13(16)15-11-8-7-10(2)12(14)9-11/h7-9H,3-6H2,1-2H3
InchiKey: ZZBBHLHOEVPZGU-UHFFFAOYSA-N
Formula: C13H18ClNO
SMILES: CCCCCC(=O)Nc1ccc(C)c(Cl)c1
Mol. weight [g/mol]: 239.74

Physical Properties

Property code	Value	Unit	Source
gf	100.27	kJ/mol	Joback Method
hf	-172.91	kJ/mol	Joback Method
hfus	33.58	kJ/mol	Joback Method
hvap	65.70	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.167		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	2031.00		NIST Webbook
rinpol	2031.00		NIST Webbook
tb	674.95	K	Joback Method
tc	885.27	K	Joback Method
tf	420.24	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.00	J/mol×K	674.95	Joback Method
cpg	511.33	J/mol×K	710.00	Joback Method
cpg	524.79	J/mol×K	745.06	Joback Method
cpg	537.41	J/mol×K	780.11	Joback Method
cpg	549.23	J/mol×K	815.16	Joback Method
cpg	560.28	J/mol×K	850.22	Joback Method
cpg	570.59	J/mol×K	885.27	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=R149116&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