3'-chloro,4'-methylbutyroanilide

Inchi: InChI=1S/C11H14ClNO/c1-3-4-11(14)13-9-6-5-8(2)10(12)7-9/h5-7H,3-4H2,1-2H3,(H,13,1
InchiKey: CMVIYVQUKDZLRB-UHFFFAOYSA-N
Formula: C11H14ClNO
SMILES: CCCC(=O)Nc1ccc(C)c(Cl)c1
Mol. weight [g/mol]: 211.69

Physical Properties

Property code	Value	Unit	Source
gf	83.43	kJ/mol	Joback Method
hf	-131.63	kJ/mol	Joback Method
hfus	28.40	kJ/mol	Joback Method
hvap	61.25	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.387		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	629.19	K	Joback Method
tc	846.41	K	Joback Method
tf	397.70	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.34	J/mol×K	629.19	Joback Method
cpg	409.49	J/mol×K	665.39	Joback Method
cpg	421.83	J/mol×K	701.60	Joback Method
cpg	433.38	J/mol×K	737.80	Joback Method
cpg	444.18	J/mol×K	774.00	Joback Method
cpg	454.25	J/mol×K	810.20	Joback Method
cpg	463.63	J/mol×K	846.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149101&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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