3'-chloro,4'-methylvaleroanilide

Inchi: InChI=1S/C12H16ClNO/c1-3-4-5-12(15)14-10-7-6-9(2)11(13)8-10/h6-8H,3-5H2,1-2H3,(H
InchiKey: MUDBOJKTKQUTFU-UHFFFAOYSA-N
Formula: C12H16ClNO
SMILES: CCCCC(=O)Nc1ccc(C)c(Cl)c1
Mol. weight [g/mol]: 225.72

Physical Properties

Property code	Value	Unit	Source
gf	91.85	kJ/mol	Joback Method
hf	-152.27	kJ/mol	Joback Method
hfus	30.99	kJ/mol	Joback Method
hvap	63.47	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.777		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1932.00		NIST Webbook
tb	652.07	K	Joback Method
tc	865.67	K	Joback Method
tf	408.97	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.95	J/mol×K	652.07	Joback Method
cpg	459.74	J/mol×K	687.67	Joback Method
cpg	472.68	J/mol×K	723.27	Joback Method
cpg	484.81	J/mol×K	758.87	Joback Method
cpg	496.16	J/mol×K	794.47	Joback Method
cpg	506.75	J/mol×K	830.07	Joback Method
cpg	516.63	J/mol×K	865.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149161&Units=SI

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