3',4'-Dichlorovaleroanilide

Inchi: InChI=1S/C11H13Cl2NO/c1-2-3-4-11(15)14-8-5-6-9(12)10(13)7-8/h5-7H,2-4H2,1H3,(H,1
InchiKey: BMSSRNRFXGWOEZ-UHFFFAOYSA-N
Formula: C11H13Cl2NO
SMILES: CCCCC(=O)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 246.13

Physical Properties

Property code	Value	Unit	Source
gf	71.50	kJ/mol	Joback Method
hf	-147.37	kJ/mol	Joback Method
hfus	32.60	kJ/mol	Joback Method
hvap	65.63	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.122		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	2030.00		NIST Webbook
tb	666.62	K	Joback Method
tc	887.14	K	Joback Method
tf	427.62	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.93	J/mol×K	666.62	Joback Method
cpg	433.11	J/mol×K	703.37	Joback Method
cpg	444.48	J/mol×K	740.13	Joback Method
cpg	455.07	J/mol×K	776.88	Joback Method
cpg	464.92	J/mol×K	813.64	Joback Method
cpg	474.06	J/mol×K	850.39	Joback Method
cpg	482.52	J/mol×K	887.14	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=R149087&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