3',4'-Dichlorocaproanilide

Inchi: InChI=1S/C12H15Cl2NO/c1-2-3-4-5-12(16)15-9-6-7-10(13)11(14)8-9/h6-8H,2-5H2,1H3,(
InchiKey: UHNACMYDEPKBKS-UHFFFAOYSA-N
Formula: C12H15Cl2NO
SMILES: CCCCCC(=O)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 260.16

Physical Properties

Property code	Value	Unit	Source
gf	79.92	kJ/mol	Joback Method
hf	-168.01	kJ/mol	Joback Method
hfus	35.19	kJ/mol	Joback Method
hvap	67.86	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.512		Crippen Method
mcvol	192.210	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook
tb	689.50	K	Joback Method
tc	906.36	K	Joback Method
tf	438.89	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.24	J/mol×K	689.50	Joback Method
cpg	484.02	J/mol×K	725.64	Joback Method
cpg	495.96	J/mol×K	761.79	Joback Method
cpg	507.10	J/mol×K	797.93	Joback Method
cpg	517.47	J/mol×K	834.08	Joback Method
cpg	527.12	J/mol×K	870.22	Joback Method
cpg	536.06	J/mol×K	906.36	Joback Method

Sources

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=R149047&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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