3',4'-Dichlorocyclohexanecarboxanilide

Inchi: InChI=1S/C13H15Cl2NO/c14-11-7-6-10(8-12(11)15)16-13(17)9-4-2-1-3-5-9/h6-9H,1-5H2
InchiKey: QNLPPYRKEBGGHV-UHFFFAOYSA-N
Formula: C13H15Cl2NO
SMILES: O=C(Nc1ccc(Cl)c(Cl)c1)C1CCCCC1
Mol. weight [g/mol]: 272.17
CAS: 15907-85-4

Physical Properties

Property code	Value	Unit	Source
gf	112.79	kJ/mol	Joback Method
hf	-134.33	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	70.51	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.512		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
tb	731.93	K	Joback Method
tc	979.89	K	Joback Method
tf	457.54	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.43	J/mol×K	731.93	Joback Method
cpg	529.91	J/mol×K	773.26	Joback Method
cpg	544.07	J/mol×K	814.58	Joback Method
cpg	556.96	J/mol×K	855.91	Joback Method
cpg	568.65	J/mol×K	897.24	Joback Method
cpg	579.21	J/mol×K	938.56	Joback Method
cpg	588.69	J/mol×K	979.89	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=C15907854&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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