4-Chloro-2-[(2-chloro-4-nitro-phenyl)carbamoyl]pl acetate

Inchi: InChI=1S/C15H10Cl2N2O5/c1-8(20)24-14-5-2-9(16)6-11(14)15(21)18-13-4-3-10(19(22)2

InchiKey: HCXKJODUWBFNTM-UHFFFAOYSA-N

Formula: C15H10Cl2N2O5

SMILES: CC(=O)Oc1ccc(Cl)cc1C(=O)Nc1ccc([N+](=O)[O-])cc1Cl

Mol. weight [g/mol]: 369.16

Physical Properties

Property code	Value	Unit	Source
gf	-0.04	kJ/mol	Joback Method
hf	-271.90	kJ/mol	Joback Method
hfus	50.37	kJ/mol	Joback Method
hvap	103.88	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.079		Crippen Method
mcvol	235.580	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	1022.91	K	Joback Method
tc	1286.08	K	Joback Method
tf	739.93	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.99	J/mol×K	1022.91	Joback Method
cpg	650.36	J/mol×K	1066.77	Joback Method
cpg	655.56	J/mol×K	1110.63	Joback Method
cpg	659.64	J/mol×K	1154.49	Joback Method
cpg	662.63	J/mol×K	1198.35	Joback Method
cpg	664.60	J/mol×K	1242.21	Joback Method
cpg	665.59	J/mol×K	1286.08	Joback Method

Sources

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=U373198&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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