2-Chlorobenzoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C13H8ClNO4/c14-12-4-2-1-3-11(12)13(16)19-10-7-5-9(6-8-10)15(17)18/h1-8H
InchiKey: LYQCUKYZFNQYEG-UHFFFAOYSA-N
Formula: C13H8ClNO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1ccccc1Cl
Mol. weight [g/mol]: 277.66

Physical Properties

Property code	Value	Unit	Source
gf	53.84	kJ/mol	Joback Method
hf	-132.83	kJ/mol	Joback Method
hfus	35.07	kJ/mol	Joback Method
hvap	80.54	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.467		Crippen Method
mcvol	183.610	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	825.72	K	Joback Method
tc	1095.18	K	Joback Method
tf	559.84	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.52	J/mol×K	825.72	Joback Method
cpg	485.78	J/mol×K	870.63	Joback Method
cpg	494.85	J/mol×K	915.54	Joback Method
cpg	502.79	J/mol×K	960.45	Joback Method
cpg	509.67	J/mol×K	1005.36	Joback Method
cpg	515.53	J/mol×K	1050.27	Joback Method
cpg	520.45	J/mol×K	1095.18	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=U307820&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