4-Nitrobenzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C13H7Cl2NO4/c14-11-6-5-10(7-12(11)15)20-13(17)8-1-3-9(4-2-8)16(18)19/h1-
InchiKey: LXEDUJYAENAZGC-UHFFFAOYSA-N
Formula: C13H7Cl2NO4
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 312.11

Physical Properties

Property code	Value	Unit	Source
gf	32.28	kJ/mol	Joback Method
hf	-160.04	kJ/mol	Joback Method
hfus	38.88	kJ/mol	Joback Method
hvap	85.59	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.121		Crippen Method
mcvol	195.850	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	2465.00		NIST Webbook
rinpol	2465.00		NIST Webbook
tb	868.13	K	Joback Method
tc	1139.27	K	Joback Method
tf	602.28	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.43	J/mol×K	868.13	Joback Method
cpg	500.28	J/mol×K	913.32	Joback Method
cpg	508.00	J/mol×K	958.51	Joback Method
cpg	514.63	J/mol×K	1003.70	Joback Method
cpg	520.24	J/mol×K	1048.89	Joback Method
cpg	524.88	J/mol×K	1094.08	Joback Method
cpg	528.58	J/mol×K	1139.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308013&Units=SI
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

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