Benzoic acid, (4-chloro-3-nitrophenyl)methyl ester

Inchi: InChI=1S/C14H10ClNO4/c15-12-7-6-10(8-13(12)16(18)19)9-20-14(17)11-4-2-1-3-5-11/h
InchiKey: PKYSTVRAGCEVSB-UHFFFAOYSA-N
Formula: C14H10ClNO4
SMILES: O=C(OCc1ccc(Cl)c([N+](=O)[O-])c1)c1ccccc1
Mol. weight [g/mol]: 291.69

Physical Properties

Property code	Value	Unit	Source
gf	62.26	kJ/mol	Joback Method
hf	-153.47	kJ/mol	Joback Method
hfus	37.66	kJ/mol	Joback Method
hvap	82.77	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.605		Crippen Method
mcvol	197.700	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	2442.00		NIST Webbook
rinpol	2442.00		NIST Webbook
tb	848.60	K	Joback Method
tc	1112.08	K	Joback Method
tf	571.11	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.71	J/mol×K	848.60	Joback Method
cpg	539.35	J/mol×K	892.51	Joback Method
cpg	548.80	J/mol×K	936.43	Joback Method
cpg	557.12	J/mol×K	980.34	Joback Method
cpg	564.36	J/mol×K	1024.25	Joback Method
cpg	570.60	J/mol×K	1068.17	Joback Method
cpg	575.89	J/mol×K	1112.08	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=U368746&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