Methyl 2-chloro-4-nitrobenzoate

Other names: Benzoic acid, 2-chloro-4-nitro-, methyl ester
Inchi: InChI=1S/C8H6ClNO4/c1-14-8(11)6-3-2-5(10(12)13)4-7(6)9/h2-4H,1H3
InchiKey: PICNSXCJRMYANX-UHFFFAOYSA-N
Formula: C8H6ClNO4
SMILES: COC(=O)c1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]: 215.59
CAS: 13324-11-3

Physical Properties

Property code	Value	Unit	Source
gf	-100.67	kJ/mol	Joback Method
hf	-266.16	kJ/mol	Joback Method
hfus	28.08	kJ/mol	Joback Method
hvap	67.13	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.035		Crippen Method
mcvol	136.920	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	684.64	K	Joback Method
tc	935.81	K	Joback Method
tf	477.07	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.03	J/mol×K	684.64	Joback Method
cpg	326.49	J/mol×K	726.50	Joback Method
cpg	335.16	J/mol×K	768.36	Joback Method
cpg	343.06	J/mol×K	810.23	Joback Method
cpg	350.20	J/mol×K	852.09	Joback Method
cpg	356.59	J/mol×K	893.95	Joback Method
cpg	362.23	J/mol×K	935.81	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=C13324113&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume