Formic acid, (2-chloro-5-nitrophenyl)methyl ester

Inchi: InChI=1S/C8H6ClNO4/c9-8-2-1-7(10(12)13)3-6(8)4-14-5-11/h1-3,5H,4H2
InchiKey: SKGAPYJBJWXFLP-UHFFFAOYSA-N
Formula: C8H6ClNO4
SMILES: O=COCc1cc([N+](=O)[O-])ccc1Cl
Mol. weight [g/mol]: 215.59

Physical Properties

Property code	Value	Unit	Source
gf	-71.27	kJ/mol	Joback Method
hf	-239.16	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	67.11	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	1.921		Crippen Method
mcvol	136.920	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
rinpol	1683.00		NIST Webbook
tb	679.43	K	Joback Method
tc	925.25	K	Joback Method
tf	469.14	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.30	J/mol×K	679.43	Joback Method
cpg	327.51	J/mol×K	720.40	Joback Method
cpg	335.98	J/mol×K	761.37	Joback Method
cpg	343.72	J/mol×K	802.34	Joback Method
cpg	350.74	J/mol×K	843.31	Joback Method
cpg	357.06	J/mol×K	884.28	Joback Method
cpg	362.69	J/mol×K	925.25	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=U368740&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

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