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

Inchi: InChI=1S/C9H8ClNO4/c1-6(12)15-5-7-4-8(10)2-3-9(7)11(13)14/h2-4H,5H2,1H3
InchiKey: CXXIIBNSKGJPIM-UHFFFAOYSA-N
Formula: C9H8ClNO4
SMILES: CC(=O)OCc1cc(Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 229.62

Physical Properties

Property code	Value	Unit	Source
gf	-92.25	kJ/mol	Joback Method
hf	-286.80	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	69.36	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.311		Crippen Method
mcvol	151.010	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1696.00		NIST Webbook
rinpol	1696.00		NIST Webbook
tb	707.52	K	Joback Method
tc	953.17	K	Joback Method
tf	488.34	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.58	J/mol×K	707.52	Joback Method
cpg	375.84	J/mol×K	748.46	Joback Method
cpg	385.27	J/mol×K	789.40	Joback Method
cpg	393.87	J/mol×K	830.35	Joback Method
cpg	401.66	J/mol×K	871.29	Joback Method
cpg	408.66	J/mol×K	912.23	Joback Method
cpg	414.88	J/mol×K	953.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368733&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

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