Acetic acid, chloro-, p-nitrophenyl ester

Inchi: InChI=1S/C8H6ClNO4/c9-5-8(11)14-7-3-1-6(2-4-7)10(12)13/h1-4H,5H2
InchiKey: DYFFUJNIXCDLOR-UHFFFAOYSA-N
Formula: C8H6ClNO4
SMILES: O=C(CCl)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 215.59
CAS: 777-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-91.04	kJ/mol	Joback Method
hf	-254.69	kJ/mol	Joback Method
hfus	28.47	kJ/mol	Joback Method
hvap	66.47	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.739		Crippen Method
mcvol	136.920	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
tb	679.66	K	Joback Method
tc	929.97	K	Joback Method
tf	464.55	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.83	J/mol×K	679.66	Joback Method
cpg	328.44	J/mol×K	721.38	Joback Method
cpg	337.23	J/mol×K	763.10	Joback Method
cpg	345.21	J/mol×K	804.82	Joback Method
cpg	352.41	J/mol×K	846.53	Joback Method
cpg	358.85	J/mol×K	888.25	Joback Method
cpg	364.55	J/mol×K	929.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C777844&Units=SI&Mask=3FFF

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

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