Dichloroacetic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C8H5Cl2NO4/c9-7(10)8(12)15-6-3-1-5(2-4-6)11(13)14/h1-4,7H
InchiKey: PXRGBMOGEXCISN-UHFFFAOYSA-N
Formula: C8H5Cl2NO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)C(Cl)Cl
Mol. weight [g/mol]: 250.04

Physical Properties

Property code	Value	Unit	Source
gf	-105.41	kJ/mol	Joback Method
hf	-275.71	kJ/mol	Joback Method
hfus	29.15	kJ/mol	Joback Method
hvap	70.47	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.304		Crippen Method
mcvol	149.160	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	1707.00		NIST Webbook
tb	716.65	K	Joback Method
tc	974.41	K	Joback Method
tf	479.47	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.71	J/mol×K	716.65	Joback Method
cpg	347.49	J/mol×K	759.61	Joback Method
cpg	355.40	J/mol×K	802.57	Joback Method
cpg	362.46	J/mol×K	845.53	Joback Method
cpg	368.71	J/mol×K	888.49	Joback Method
cpg	374.17	J/mol×K	931.45	Joback Method
cpg	378.87	J/mol×K	974.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307589&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

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