Carbonic acid, 2,2,2-trichloroethyl 4-nitrophenyl ester

Inchi: InChI=1S/C9H6Cl3NO5/c10-9(11,12)5-17-8(14)18-7-3-1-6(2-4-7)13(15)16/h1-4H,5H2
InchiKey: SDHPSMBWDAIAHJ-UHFFFAOYSA-N
Formula: C9H6Cl3NO5
SMILES: O=C(OCC(Cl)(Cl)Cl)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 314.51

Physical Properties

Property code	Value	Unit	Source
gf	-208.64	kJ/mol	Joback Method
hf	-447.78	kJ/mol	Joback Method
hfus	33.23	kJ/mol	Joback Method
hvap	78.58	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.480		Crippen Method
mcvol	181.360	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	2086.00		NIST Webbook
rinpol	2086.00		NIST Webbook
tb	796.59	K	Joback Method
tc	1055.15	K	Joback Method
tf	560.31	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.74	J/mol×K	796.59	Joback Method
cpg	438.77	J/mol×K	839.68	Joback Method
cpg	445.84	J/mol×K	882.78	Joback Method
cpg	452.01	J/mol×K	925.87	Joback Method
cpg	457.30	J/mol×K	968.96	Joback Method
cpg	461.79	J/mol×K	1012.06	Joback Method
cpg	465.50	J/mol×K	1055.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357905&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