2,2,2-Trichloro-1-cyanoethyl 4-chlorobenzoate

Inchi: InChI=1S/C10H5Cl4NO2/c11-7-3-1-6(2-4-7)9(16)17-8(5-15)10(12,13)14/h1-4,8H
InchiKey: GXQADAOVOZXMNA-UHFFFAOYSA-N
Formula: C10H5Cl4NO2
SMILES: N#CC(OC(=O)c1ccc(Cl)cc1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 312.96
CAS: 101166-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-11.96	kJ/mol	Joback Method
hf	-181.58	kJ/mol	Joback Method
hfus	25.45	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.759		Crippen Method
mcvol	185.780	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
tb	784.28	K	Joback Method
tc	1040.84	K	Joback Method
tf	485.65	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.27	J/mol×K	784.28	Joback Method
cpg	411.40	J/mol×K	827.04	Joback Method
cpg	417.72	J/mol×K	869.80	Joback Method
cpg	423.32	J/mol×K	912.56	Joback Method
cpg	428.25	J/mol×K	955.32	Joback Method
cpg	432.58	J/mol×K	998.08	Joback Method
cpg	436.38	J/mol×K	1040.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101166965&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume