3-(2,2,2-Trichloro-1,1-dimethylethoxy)-2-benzofura

Inchi: InChI=1S/C12H11Cl3O3/c1-11(2,12(13,14)15)18-10-8-6-4-3-5-7(8)9(16)17-10/h3-6,10H,
InchiKey: XFHFPSJKJWQYGG-UHFFFAOYSA-N
Formula: C12H11Cl3O3
SMILES: CC(C)(OC1OC(=O)c2ccccc21)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 309.57
CAS: 100062-58-6

Physical Properties

Property code	Value	Unit	Source
gf	-130.13	kJ/mol	Joback Method
hf	-459.79	kJ/mol	Joback Method
hfus	25.06	kJ/mol	Joback Method
hvap	66.89	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.021		Crippen Method
mcvol	195.350	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
tb	735.38	K	Joback Method
tc	996.51	K	Joback Method
tf	493.50	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.57	J/mol×K	735.38	Joback Method
cpg	512.46	J/mol×K	778.90	Joback Method
cpg	524.13	J/mol×K	822.42	Joback Method
cpg	534.70	J/mol×K	865.94	Joback Method
cpg	544.28	J/mol×K	909.46	Joback Method
cpg	552.97	J/mol×K	952.99	Joback Method
cpg	560.88	J/mol×K	996.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100062586&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume