1-(2,2-Dimethyl-1,3-dioxolan-4-yl)-2-methoxy-2-ox
3-chlorobenzoate

Inchi: InChI=1S/C15H17ClO6/c1-15(2)20-8-11(22-15)12(14(18)19-3)21-13(17)9-5-4-6-10(16)7-

InchiKey: ZKKWYJBTVAEXOY-UHFFFAOYSA-N

Formula: C15H17ClO6

SMILES: COC(=O)C(OC(=O)c1cccc(Cl)c1)C1COC(C)(C)O1

Mol. weight [g/mol]: 328.75

Physical Properties

Property code	Value	Unit	Source
gf	-452.90	kJ/mol	Joback Method
hf	-847.11	kJ/mol	Joback Method
hfus	39.17	kJ/mol	Joback Method
hvap	82.05	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.190		Crippen Method
mcvol	226.450	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	828.58	K	Joback Method
tc	1064.64	K	Joback Method
tf	540.69	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.75	J/mol×K	828.58	Joback Method
cpg	684.92	J/mol×K	867.92	Joback Method
cpg	699.44	J/mol×K	907.27	Joback Method
cpg	713.43	J/mol×K	946.61	Joback Method
cpg	727.02	J/mol×K	985.95	Joback Method
cpg	740.33	J/mol×K	1025.30	Joback Method
cpg	753.49	J/mol×K	1064.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373578&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