3,4,5-Trimethoxybenzoyl chloride

Other names:	Benzoyl chloride, 3,4,5-trimethoxy-
	Tri-O-methylgalloyl chloride
	Trimethylgalloyl chloride
Inchi:	InChI=1S/C10H11ClO4/c1-13-7-4-6(10(11)12)5-8(14-2)9(7)15-3/h4-5H,1-3H3
InchiKey:	BUHYMJLFRZAFBF-UHFFFAOYSA-N
Formula:	C10H11ClO4
SMILES:	COc1cc(C(=O)Cl)cc(OC)c1OC
Mol. weight [g/mol]:	230.65
CAS:	4521-61-3

Physical Properties

Property code	Value	Unit	Source
gf	-339.01	kJ/mol	Joback Method
hf	-572.59	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	60.48	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.091		Crippen Method
mcvol	159.420	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	628.38	K	Joback Method
tc	843.30	K	Joback Method
tf	412.98	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.96	J/mol×K	628.38	Joback Method
cpg	382.73	J/mol×K	664.20	Joback Method
cpg	393.90	J/mol×K	700.02	Joback Method
cpg	404.46	J/mol×K	735.84	Joback Method
cpg	414.37	J/mol×K	771.66	Joback Method
cpg	423.60	J/mol×K	807.48	Joback Method

cpg	432.13	J/mol×K	843.30	Joback Method
dvisc	0.0006375	Pa×s	412.98	Joback Method
dvisc	0.0004399	Pa×s	448.88	Joback Method
dvisc	0.0003207	Pa×s	484.78	Joback Method
dvisc	0.0002442	Pa×s	520.68	Joback Method
dvisc	0.0001927	Pa×s	556.58	Joback Method
dvisc	0.0001564	Pa×s	592.48	Joback Method
dvisc	0.0001300	Pa×s	628.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	2.40	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521613&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume