Isopropyl 3-chloro-5-formyl-4,6-dihydroxy-2-methylbenzoat

Inchi: InChI=1S/C12H13ClO5/c1-5(2)18-12(17)8-6(3)9(13)11(16)7(4-14)10(8)15/h4-5,15-16H,1

InchiKey: NKIVWTXLVQIYGX-UHFFFAOYSA-N

Formula: C12H13ClO5

SMILES: Cc1c(Cl)c(O)c(C=O)c(O)c1C(=O)OC(C)C

Mol. weight [g/mol]: 272.68

CAS: 959266-90-1

Physical Properties

Property code	Value	Unit	Source
gf	-523.37	kJ/mol	Joback Method
hf	-794.91	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	92.47	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.437		Crippen Method
mcvol	189.170	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	2001.20		NIST Webbook
rinpol	2001.20		NIST Webbook
tb	838.76	K	Joback Method
tc	1072.70	K	Joback Method
tf	641.50	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.94	J/mol×K	838.76	Joback Method
cpg	532.12	J/mol×K	877.75	Joback Method
cpg	542.03	J/mol×K	916.74	Joback Method
cpg	551.76	J/mol×K	955.73	Joback Method
cpg	561.41	J/mol×K	994.72	Joback Method
cpg	571.10	J/mol×K	1033.71	Joback Method
cpg	580.92	J/mol×K	1072.70	Joback Method

dvisc	0.0000069	Pa×s	641.50	Joback Method
dvisc	0.0000040	Pa×s	674.38	Joback Method
dvisc	0.0000024	Pa×s	707.25	Joback Method
dvisc	0.0000016	Pa×s	740.13	Joback Method
dvisc	0.0000010	Pa×s	773.01	Joback Method
dvisc	0.0000007	Pa×s	805.88	Joback Method
dvisc	0.0000005	Pa×s	838.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959266901&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume