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

Inchi: InChI=1S/C11H11ClO5/c1-3-17-11(16)7-5(2)8(12)10(15)6(4-13)9(7)14/h4,14-15H,3H2,1-

InchiKey: QWBSIYICLWCIDS-UHFFFAOYSA-N

Formula: C11H11ClO5

SMILES: CCOC(=O)c1c(C)c(Cl)c(O)c(C=O)c1O

Mol. weight [g/mol]: 258.65

CAS: 57857-81-5

Physical Properties

Property code	Value	Unit	Source
gf	-529.35	kJ/mol	Joback Method
hf	-768.99	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	90.63	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.049		Crippen Method
mcvol	175.080	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
tb	816.32	K	Joback Method
tc	1050.01	K	Joback Method
tf	645.23	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.30	J/mol×K	816.32	Joback Method
cpg	513.12	J/mol×K	1011.06	Joback Method
cpg	504.26	J/mol×K	972.11	Joback Method
cpg	495.45	J/mol×K	933.16	Joback Method
cpg	486.59	J/mol×K	894.22	Joback Method
cpg	477.57	J/mol×K	855.27	Joback Method
cpg	522.11	J/mol×K	1050.01	Joback Method
dvisc	0.0000007	Pa×s	816.32	Joback Method
dvisc	0.0000010	Pa×s	787.80	Joback Method

dvisc	0.0000014	Pa×s	759.29	Joback Method
dvisc	0.0000020	Pa×s	730.77	Joback Method
dvisc	0.0000029	Pa×s	702.26	Joback Method
dvisc	0.0000044	Pa×s	673.75	Joback Method
dvisc	0.0000069	Pa×s	645.23	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=C57857815&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume