Isopropyl 3-chloro-6-hydroxy-4-methoxy-2-methylbenzoate

Inchi: InChI=1S/C12H15ClO4/c1-6(2)17-12(15)10-7(3)11(13)9(16-4)5-8(10)14/h5-6,14H,1-4H3

InchiKey: KJHOFASQYUCZPN-UHFFFAOYSA-N

Formula: C12H15ClO4

SMILES: COc1cc(O)c(C(=O)OC(C)C)c(C)c1Cl

Mol. weight [g/mol]: 258.70

Physical Properties

Property code	Value	Unit	Source
gf	-374.23	kJ/mol	Joback Method
hf	-664.24	kJ/mol	Joback Method
hfus	30.14	kJ/mol	Joback Method
hvap	75.14	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.928		Crippen Method
mcvol	187.600	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1904.80		NIST Webbook
rinpol	1904.80		NIST Webbook
tb	731.90	K	Joback Method
tc	954.64	K	Joback Method
tf	510.01	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.23	J/mol×K	731.90	Joback Method
cpg	548.68	J/mol×K	917.52	Joback Method
cpg	539.07	J/mol×K	880.39	Joback Method
cpg	528.85	J/mol×K	843.27	Joback Method
cpg	517.99	J/mol×K	806.15	Joback Method
cpg	506.47	J/mol×K	769.02	Joback Method
cpg	557.71	J/mol×K	954.64	Joback Method
dvisc	0.0000098	Pa×s	731.90	Joback Method

dvisc	0.0000136	Pa×s	694.92	Joback Method
dvisc	0.0000196	Pa×s	657.94	Joback Method
dvisc	0.0000296	Pa×s	620.96	Joback Method
dvisc	0.0000470	Pa×s	583.97	Joback Method
dvisc	0.0000794	Pa×s	546.99	Joback Method
dvisc	0.0001447	Pa×s	510.01	Joback Method

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=U413423&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume