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

Inchi: InChI=1S/C11H13ClO4/c1-4-16-11(14)9-6(2)10(12)8(15-3)5-7(9)13/h5,13H,4H2,1-3H3
InchiKey: DTAMIZHNUNMPJD-UHFFFAOYSA-N
Formula: C11H13ClO4
SMILES: CCOC(=O)c1c(O)cc(OC)c(Cl)c1C
Mol. weight [g/mol]: 244.67
CAS: 57074-24-5

Physical Properties

Property code	Value	Unit	Source
gf	-380.21	kJ/mol	Joback Method
hf	-638.32	kJ/mol	Joback Method
hfus	31.07	kJ/mol	Joback Method
hvap	73.31	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.539		Crippen Method
mcvol	173.510	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1874.70		NIST Webbook
rinpol	1874.70		NIST Webbook
tb	709.46	K	Joback Method
tc	931.85	K	Joback Method
tf	513.74	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.40	J/mol×K	709.46	Joback Method
cpg	493.10	J/mol×K	894.78	Joback Method
cpg	484.11	J/mol×K	857.72	Joback Method
cpg	474.57	J/mol×K	820.65	Joback Method
cpg	464.46	J/mol×K	783.59	Joback Method
cpg	453.75	J/mol×K	746.52	Joback Method
cpg	501.57	J/mol×K	931.85	Joback Method

dvisc	0.0000130	Pa×s	709.46	Joback Method
dvisc	0.0000176	Pa×s	676.84	Joback Method
dvisc	0.0000244	Pa×s	644.22	Joback Method
dvisc	0.0000352	Pa×s	611.60	Joback Method
dvisc	0.0000527	Pa×s	578.98	Joback Method
dvisc	0.0000830	Pa×s	546.36	Joback Method
dvisc	0.0001385	Pa×s	513.74	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=C57074245&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