Ethyl 2,4-dihydroxy-3,6-dimethylbenzoate

Inchi: InChI=1S/C11H14O4/c1-4-15-11(14)9-6(2)5-8(12)7(3)10(9)13/h5,12-13H,4H2,1-3H3
InchiKey: VJLLNFDLMWPNBN-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: CCOC(=O)c1c(C)cc(O)c(C)c1O
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
hf	-724.35	kJ/mol	Cheméo Relay (1.0)
hfus	31.86	kJ/mol	Joback Method
hvap	92.81	kJ/mol	Cheméo Relay (1.0)
ie	7.87	eV	Cheméo Relay (1.0)
log10ws	-2.63		Cheméo Relay (1.0)
logp	1.891		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	1796.70		NIST Webbook
rinpol	1796.70		NIST Webbook
tb	571.13	K	Cheméo Relay (1.0)
tf	402.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.87	J/mol×K	725.25	Joback Method
cpg	453.01	J/mol×K	763.47	Joback Method
cpg	463.65	J/mol×K	801.68	Joback Method
cpg	473.88	J/mol×K	839.90	Joback Method
cpg	483.81	J/mol×K	878.12	Joback Method
cpg	493.53	J/mol×K	916.33	Joback Method
cpg	503.15	J/mol×K	954.55	Joback Method
dvisc	0.0000200	Pa×s	560.79	Joback Method
dvisc	0.0000115	Pa×s	588.20	Joback Method
dvisc	0.0000069	Pa×s	615.61	Joback Method

dvisc	0.0000044	Pa×s	643.02	Joback Method
dvisc	0.0000029	Pa×s	670.43	Joback Method
dvisc	0.0000019	Pa×s	697.84	Joback Method
dvisc	0.0000013	Pa×s	725.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31581325&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
tf: Normal melting (fusion) point