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

Other names: Ethyl 2-hydroxy-4-methoxy-6-methylbenzoate
Inchi: InChI=1S/C11H14O4/c1-4-15-11(13)10-7(2)5-8(14-3)6-9(10)12/h5-6,12H,4H2,1-3H3
InchiKey: PJOOIAZRUIIQMU-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: CCOC(=O)c1c(C)cc(OC)cc1O
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
hf	-670.03	kJ/mol	Cheméo Relay (1.0)
hfus	27.27	kJ/mol	Joback Method
ie	7.85	eV	Cheméo Relay (1.0)
log10ws	-3.39		Cheméo Relay (1.0)
logp	1.886		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
rinpol	1680.10		NIST Webbook
tb	561.59	K	Cheméo Relay (1.0)
tf	329.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.53	J/mol×K	667.05	Joback Method
cpg	432.84	J/mol×K	703.47	Joback Method
cpg	444.47	J/mol×K	739.89	Joback Method
cpg	455.46	J/mol×K	776.31	Joback Method
cpg	465.83	J/mol×K	812.72	Joback Method
cpg	475.62	J/mol×K	849.14	Joback Method
cpg	484.86	J/mol×K	885.56	Joback Method
dvisc	0.0002436	Pa×s	471.30	Joback Method
dvisc	0.0001353	Pa×s	503.93	Joback Method
dvisc	0.0000807	Pa×s	536.55	Joback Method
dvisc	0.0000511	Pa×s	569.17	Joback Method
dvisc	0.0000340	Pa×s	601.80	Joback Method

dvisc	0.0000236	Pa×s	634.42	Joback Method
dvisc	0.0000170	Pa×s	667.05	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6110367&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point