Benzoic acid, 3,4-dihydroxy-, ethyl ester

Other names:	Ethyl protocatechuate
	Protocatechuic acid ethyl ester
	Benzoic acid, 3,4-dihydroxy-, ethyl ester
Inchi:	InChI=1S/C9H10O4/c1-2-13-9(12)6-3-4-7(10)8(11)5-6/h3-5,10-11H,2H2,1H3
InchiKey:	KBPUBCVJHFXPOC-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	CCOC(=O)c1ccc(O)c(O)c1
Mol. weight [g/mol]:	182.18

Physical Properties

Property code	Value	Unit	Source
af	0.7707		Cheméo Relay (1.0)
hf	-674.09	kJ/mol	Cheméo Relay (1.0)
hfus	27.46	kJ/mol	Joback Method
hvap	99.75	kJ/mol	Cheméo Relay (1.0)
ie	8.49	eV	Cheméo Relay (1.0)
log10ws	-1.87		Cheméo Relay (1.0)
logp	1.274		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	5051.40	kPa	Joback Method
tb	565.82	K	Cheméo Relay (1.0)
tc	789.52	K	Cheméo Relay (1.0)
tf	407.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.64	J/mol×K	669.53	Joback Method
cpg	356.36	J/mol×K	708.97	Joback Method
cpg	365.48	J/mol×K	748.41	Joback Method
cpg	374.12	J/mol×K	787.85	Joback Method
cpg	382.41	J/mol×K	827.29	Joback Method
cpg	390.46	J/mol×K	866.73	Joback Method
cpg	398.39	J/mol×K	906.17	Joback Method

dvisc	0.0000545	Pa×s	513.21	Joback Method
dvisc	0.0000293	Pa×s	539.26	Joback Method
dvisc	0.0000167	Pa×s	565.32	Joback Method
dvisc	0.0000100	Pa×s	591.37	Joback Method
dvisc	0.0000062	Pa×s	617.42	Joback Method
dvisc	0.0000041	Pa×s	643.48	Joback Method
dvisc	0.0000027	Pa×s	669.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3943893&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

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.