ethyl 2-hydroxy-3-phenylpropanoate

Other names: Propanoic acid, 2-hydroxy-3-phenyl, ethyl ester
ethyl phenyllactate
Inchi: InChI=1S/C11H14O3/c1-2-14-11(13)10(12)8-9-6-4-3-5-7-9/h3-7,10,12H,2,8H2,1H3
InchiKey: HBOGUIFRIAXYNB-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CCOC(=O)C(O)Cc1ccccc1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	-219.03	kJ/mol	Joback Method
hf	-436.15	kJ/mol	Joback Method
hfus	21.64	kJ/mol	Joback Method
hvap	67.80	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.153		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1445.00		NIST Webbook
ripol	2249.00		NIST Webbook
ripol	2315.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2249.00		NIST Webbook
tb	645.79	K	Joback Method
tc	845.38	K	Joback Method
tf	358.13	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.54	J/mol×K	645.79	Joback Method
cpg	453.87	J/mol×K	812.11	Joback Method
cpg	444.56	J/mol×K	778.85	Joback Method
cpg	434.60	J/mol×K	745.58	Joback Method
cpg	423.95	J/mol×K	712.32	Joback Method
cpg	412.60	J/mol×K	679.05	Joback Method
cpg	462.54	J/mol×K	845.38	Joback Method
dvisc	0.0000540	Pa×s	645.79	Joback Method
dvisc	0.0000835	Pa×s	597.85	Joback Method
dvisc	0.0001392	Pa×s	549.90	Joback Method
dvisc	0.0002559	Pa×s	501.96	Joback Method
dvisc	0.0005350	Pa×s	454.02	Joback Method
dvisc	0.0013311	Pa×s	406.07	Joback Method
dvisc	0.0042275	Pa×s	358.13	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R252574&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume