Ethyl 3-(2-hydroxyphenyl)propanoate

Inchi: InChI=1S/C11H14O3/c1-2-14-11(13)8-7-9-5-3-4-6-10(9)12/h3-6,12H,2,7-8H2,1H3
InchiKey: HXMJMZSXBPHDKV-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CCOC(=O)CCc1ccccc1O
Mol. weight [g/mol]: 194.23
CAS: 20921-04-4

Physical Properties

Property code	Value	Unit	Source
gf	-234.39	kJ/mol	Joback Method
hf	-455.95	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.888		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1576.40		NIST Webbook
rinpol	1576.40		NIST Webbook
tb	634.67	K	Joback Method
tc	854.09	K	Joback Method
tf	424.03	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.53	J/mol×K	634.67	Joback Method
cpg	455.33	J/mol×K	817.52	Joback Method
cpg	445.32	J/mol×K	780.95	Joback Method
cpg	434.71	J/mol×K	744.38	Joback Method
cpg	423.41	J/mol×K	707.81	Joback Method
cpg	411.37	J/mol×K	671.24	Joback Method
cpg	464.78	J/mol×K	854.09	Joback Method

dvisc	0.0000257	Pa×s	634.67	Joback Method
dvisc	0.0000380	Pa×s	599.56	Joback Method
dvisc	0.0000592	Pa×s	564.46	Joback Method
dvisc	0.0000977	Pa×s	529.35	Joback Method
dvisc	0.0001730	Pa×s	494.24	Joback Method
dvisc	0.0003344	Pa×s	459.14	Joback Method
dvisc	0.0007210	Pa×s	424.03	Joback Method

Sources

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=C20921044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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