Benzeneacetic acid, 2-hydroxy-, ethyl ester

Other names: Ethyl (2-hydroxyphenyl)acetate
Inchi: InChI=1S/C10H12O3/c1-2-13-10(12)7-8-5-3-4-6-9(8)11/h3-6,11H,2,7H2,1H3
InchiKey: XTRBBJJVAIWTPL-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: CCOC(=O)Cc1ccccc1O
Mol. weight [g/mol]: 180.20
CAS: 41873-65-8

Physical Properties

Property code	Value	Unit	Source
gf	-242.81	kJ/mol	Joback Method
hf	-435.31	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.498		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
rinpol	1496.00		NIST Webbook
tb	611.79	K	Joback Method
tc	835.24	K	Joback Method
tf	412.76	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.48	J/mol×K	611.79	Joback Method
cpg	362.58	J/mol×K	649.03	Joback Method
cpg	373.90	J/mol×K	686.27	Joback Method
cpg	384.49	J/mol×K	723.51	Joback Method
cpg	394.42	J/mol×K	760.76	Joback Method
cpg	403.75	J/mol×K	798.00	Joback Method
cpg	412.55	J/mol×K	835.24	Joback Method

dvisc	0.0008548	Pa×s	412.76	Joback Method
dvisc	0.0004034	Pa×s	445.93	Joback Method
dvisc	0.0002113	Pa×s	479.10	Joback Method
dvisc	0.0001203	Pa×s	512.27	Joback Method
dvisc	0.0000734	Pa×s	545.45	Joback Method
dvisc	0.0000473	Pa×s	578.62	Joback Method
dvisc	0.0000320	Pa×s	611.79	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41873658&Units=SI

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