Benzoic acid, 4-hydroxy-, pentyl ester

Other names:	Amyl 4-hydroxybenzoate
	Benzoic acid, p-hydroxy-, pentyl ester
	NSC 309817
	Pentyl 4-hydroxybenzoate
	Pentyl p-hydroxybenzoate
	n-Amyl 4-hydroxybenzoate
	p-Hydroxybenzoic acid pentyl ester
	p-Oxybenzoesaurepentylester
Inchi:	InChI=1S/C12H16O3/c1-2-3-4-9-15-12(14)10-5-7-11(13)8-6-10/h5-8,13H,2-4,9H2,1H3
InchiKey:	ZNSSPLQZSUWFJT-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CCCCCOC(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	208.25
CAS:	6521-29-5

Physical Properties

Property code	Value	Unit	Source
gf	-225.97	kJ/mol	Joback Method
hf	-476.59	kJ/mol	Joback Method
hfus	29.45	kJ/mol	Joback Method
hvap	66.75	kJ/mol	Joback Method
log10ws	-3.81		Aqueous Solubility Prediction Method
logp	2.739		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	657.55	K	Joback Method
tc	873.24	K	Joback Method
tf	435.30	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	448.08	J/mol×K	657.55	Joback Method
cpg	461.57	J/mol×K	693.50	Joback Method
cpg	474.24	J/mol×K	729.45	Joback Method
cpg	486.16	J/mol×K	765.40	Joback Method
cpg	497.38	J/mol×K	801.34	Joback Method
cpg	507.98	J/mol×K	837.29	Joback Method
cpg	518.02	J/mol×K	873.24	Joback Method
dvisc	0.0006064	Pa×s	435.30	Joback Method
dvisc	0.0002767	Pa×s	472.34	Joback Method
dvisc	0.0001415	Pa×s	509.38	Joback Method
dvisc	0.0000793	Pa×s	546.42	Joback Method
dvisc	0.0000478	Pa×s	583.47	Joback Method
dvisc	0.0000306	Pa×s	620.51	Joback Method
dvisc	0.0000206	Pa×s	657.55	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6521295&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume