p-Pentyloxybenzoic acid

Other names:	4-n-Amyloxybenzoic acid
	4-n-pentyloxybenzoic acid
	Benzoic acid, 4-(pentyloxy)-
	Benzoic acid, p-(pentyloxy)-
	p-Pentoxybenzoic acid
	p-n-Amyloxybenzoic acid
	p-n-Pentyloxybenzoic acid
Inchi:	InChI=1S/C12H16O3/c1-2-3-4-9-15-11-7-5-10(6-8-11)12(13)14/h5-8H,2-4,9H2,1H3,(H,13
InchiKey:	OZPPUPJQRJYTNY-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CCCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	208.26

Physical Properties

Property code	Value	Unit	Source
af	0.8638		Cheméo Relay (1.0)
hf	-537.88	kJ/mol	Cheméo Relay (1.0)
hfus	2.16	kJ/mol	Thermodynamic Study of 4-n-Alkyloxybenzoic Acids
hvap	100.88	kJ/mol	Cheméo Relay (1.0)
ie	8.78	eV	Cheméo Relay (1.0)
log10ws	-3.71		Cheméo Relay (1.0)
logp	2.954		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	590.83	K	Cheméo Relay (1.0)
tc	801.09	K	Cheméo Relay (1.0)
tf	398.00 ± 1.00	K	NIST Webbook
vc	0.618	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.24	J/mol×K	674.09	Joback Method

cpg	512.85	J/mol×K	868.90	Joback Method
cpg	503.87	J/mol×K	836.43	Joback Method
cpg	494.26	J/mol×K	803.96	Joback Method
cpg	484.01	J/mol×K	771.49	Joback Method
cpg	473.10	J/mol×K	739.03	Joback Method
cpg	461.52	J/mol×K	706.56	Joback Method
dvisc	0.0001841	Pa×s	535.50	Joback Method
dvisc	0.0000478	Pa×s	674.09	Joback Method
dvisc	0.0000702	Pa×s	627.89	Joback Method
dvisc	0.0001094	Pa×s	581.70	Joback Method
dvisc	0.0018159	Pa×s	396.92	Joback Method
dvisc	0.0003419	Pa×s	489.31	Joback Method
dvisc	0.0007222	Pa×s	443.12	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermodynamic Study of 4-n-Alkyloxybenzoic Acids:	https://www.doi.org/10.1021/je900776y
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15872410&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

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
vc:	Critical Volume