p-Hexyloxybenzoic acid

Other names:	4-n-Hexyloxybenzoic acid
	Benzoic acid, 4-(hexyloxy)-
	Benzoic acid, p-(hexyloxy)-
	p-Hexoylbenzoic acid
	p-n-Hexyloxybenzoic acid
Inchi:	InChI=1S/C13H18O3/c1-2-3-4-5-10-16-12-8-6-11(7-9-12)13(14)15/h6-9H,2-5,10H2,1H3,
InchiKey:	HBQUXMZZODHFMJ-UHFFFAOYSA-N
Formula:	C13H18O3
SMILES:	CCCCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	222.28

Physical Properties

Property code	Value	Unit	Source
af	0.9024		Cheméo Relay (1.0)
hf	-558.51	kJ/mol	Cheméo Relay (1.0)
hfus	3.16	kJ/mol	Thermodynamic Study of 4-n-Alkyloxybenzoic Acids
hvap	105.04	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-4.09		Cheméo Relay (1.0)
logp	3.344		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
tb	599.14	K	Cheméo Relay (1.0)
tc	812.40	K	Cheméo Relay (1.0)
tf	407.46	K	Cheméo Relay (1.0)
vc	0.674	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.87	J/mol×K	696.97	Joback Method
cpg	513.70	J/mol×K	729.14	Joback Method
cpg	525.80	J/mol×K	761.32	Joback Method

cpg	537.20	J/mol×K	793.49	Joback Method
cpg	547.90	J/mol×K	825.67	Joback Method
cpg	557.93	J/mol×K	857.84	Joback Method
cpg	567.30	J/mol×K	890.02	Joback Method
dvisc	0.0015672	Pa×s	408.19	Joback Method
dvisc	0.0006175	Pa×s	456.32	Joback Method
dvisc	0.0002906	Pa×s	504.45	Joback Method
dvisc	0.0001560	Pa×s	552.58	Joback Method
dvisc	0.0000925	Pa×s	600.71	Joback Method
dvisc	0.0000593	Pa×s	648.84	Joback Method
dvisc	0.0000404	Pa×s	696.97	Joback Method

Sources

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=C1142398&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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