4-Heptyloxybenzoic acid

Other names:	4-n-heptyloxybenzoic acid
	Benzoic acid, 4-(heptyloxy)-
	Benzoic acid, p-(heptyloxy)-
	benzoic acid, 4-heptyloxy-
	p-Heptoxybenzoic acid
	p-Heptyloxybenzoic acid
	p-n-Heptyloxybenzoic acid
Inchi:	InChI=1S/C14H20O3/c1-2-3-4-5-6-11-17-13-9-7-12(8-10-13)14(15)16/h7-10H,2-6,11H2,1
InchiKey:	ZRVIYEJYXIDATJ-UHFFFAOYSA-N
Formula:	C14H20O3
SMILES:	CCCCCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	236.31
CAS:	15872-42-1

Physical Properties

Property code	Value	Unit	Source
gf	-200.96	kJ/mol	Joback Method
hf	-504.26	kJ/mol	Joback Method
hfus	2.11	kJ/mol	Thermodynamic Study of 4-n-Alkyloxybenzoic Acids
hvap	75.53	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.734		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
tb	719.85	K	Joback Method
tc	911.57	K	Joback Method
tf	367.00 ± 1.00	K	NIST Webbook
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.80	J/mol×K	719.85	Joback Method

cpg	567.12	J/mol×K	751.80	Joback Method
cpg	579.68	J/mol×K	783.76	Joback Method
cpg	591.50	J/mol×K	815.71	Joback Method
cpg	602.60	J/mol×K	847.66	Joback Method
cpg	613.00	J/mol×K	879.62	Joback Method
cpg	622.72	J/mol×K	911.57	Joback Method
dvisc	0.0013481	Pa×s	419.46	Joback Method
dvisc	0.0005265	Pa×s	469.52	Joback Method
dvisc	0.0002465	Pa×s	519.59	Joback Method
dvisc	0.0001318	Pa×s	569.65	Joback Method
dvisc	0.0000780	Pa×s	619.72	Joback Method
dvisc	0.0000499	Pa×s	669.78	Joback Method
dvisc	0.0000340	Pa×s	719.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15872421&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic Study of 4-n-Alkyloxybenzoic Acids:	https://www.doi.org/10.1021/je900776y
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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