4-(Hexyloxy)benzoic acid

Other names: 4-n-Hexyloxybenzoic acid
Benzoic acid, 4-(hexyloxy)-
Benzoic acid, p-(hexyloxy)-
p-Hexoylbenzoic acid
p-Hexyloxybenzoic 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

CAS: 1142-39-8

Physical Properties

Property code	Value	Unit	Source
gf	-209.38	kJ/mol	Joback Method
hf	-483.62	kJ/mol	Joback Method
hfus	3.16	kJ/mol	Thermodynamic Study of 4-n-Alkyloxybenzoic Acids
hvap	73.31	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.344		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
tb	696.97	K	Joback Method
tc	890.02	K	Joback Method
tf	408.19	K	Joback Method
vc	0.699	m3/kmol	Joback Method

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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1142398&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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