4-Octyloxybenzoic acid

Other names: 4-n-Octyloxybenzoic acid
Benzoic acid, 4-(octyloxy)-
Benzoic acid, p-(octyloxy)-
p-Octoxybenzoic acid
p-Octyloxybenzoic acid
p-n-Octyloxybenzoic acid
Inchi: InChI=1S/C15H22O3/c1-2-3-4-5-6-7-12-18-14-10-8-13(9-11-14)15(16)17/h8-11H,2-7,12H
InchiKey: IALWCYFULVHLEC-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: CCCCCCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 250.33
CAS: 2493-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-192.54	kJ/mol	Joback Method
hf	-524.90	kJ/mol	Joback Method
hfus	0.79	kJ/mol	Thermodynamic Study of 4-n-Alkyloxybenzoic Acids
hsub	163.00 ± 1.20	kJ/mol	NIST Webbook
hvap	77.76	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.124		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
tb	742.73	K	Joback Method
tc	933.61	K	Joback Method
tf	430.73	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.93	J/mol×K	742.73	Joback Method

cpg	669.07	J/mol×K	901.79	Joback Method
cpg	658.34	J/mol×K	869.98	Joback Method
cpg	646.89	J/mol×K	838.17	Joback Method
cpg	634.68	J/mol×K	806.36	Joback Method
cpg	621.70	J/mol×K	774.54	Joback Method
cpg	679.09	J/mol×K	933.61	Joback Method
dvisc	0.0000286	Pa×s	742.73	Joback Method
dvisc	0.0000420	Pa×s	690.73	Joback Method
dvisc	0.0000657	Pa×s	638.73	Joback Method
dvisc	0.0001112	Pa×s	586.73	Joback Method
dvisc	0.0002086	Pa×s	534.73	Joback Method
dvisc	0.0004478	Pa×s	482.73	Joback Method
dvisc	0.0011563	Pa×s	430.73	Joback Method

Sources

Experimental standard molar enthalpies of formation of some 4-alkoxybenzoic acids:	https://www.doi.org/10.1016/j.jct.2009.08.007
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=C2493847&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hsub:	Enthalpy of sublimation 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