4-Butoxybenzoic acid

Other names:	4-Butyloxybenzoic acid
	4-n-Butoxybenzoic acid
	Benzoic acid, p-butoxy-
	benzoic acid, 4-butoxy-
	p-Butoxybenzoic acid
	p-Butyloxybenzoic acid
	p-n-Butoxybenzoic acid
	p-n-Butyloxybenzoic acid
Inchi:	InChI=1S/C11H14O3/c1-2-3-8-14-10-6-4-9(5-7-10)11(12)13/h4-7H,2-3,8H2,1H3,(H,12,13
InchiKey:	LAUFPZPAKULAGB-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	194.23
CAS:	1498-96-0

Physical Properties

Property code	Value	Unit	Source
gf	-226.22	kJ/mol	Joback Method
hf	-442.34	kJ/mol	Joback Method
hfus	2.77	kJ/mol	Thermodynamic Study of 4-n-Alkyloxybenzoic Acids
hsub	129.00 ± 0.80	kJ/mol	NIST Webbook
hvap	68.85	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.564		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
tb	651.21	K	Joback Method
tc	848.16	K	Joback Method
tf	420.70 ± 0.10	K	NIST Webbook
tf	420.90 ± 0.50	K	NIST Webbook
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.99	J/mol×K	651.21	Joback Method
cpg	410.65	J/mol×K	684.04	Joback Method
cpg	421.65	J/mol×K	716.86	Joback Method
cpg	432.01	J/mol×K	749.69	Joback Method
cpg	441.74	J/mol×K	782.51	Joback Method
cpg	450.87	J/mol×K	815.34	Joback Method
cpg	459.39	J/mol×K	848.16	Joback Method
dvisc	0.0020963	Pa×s	385.65	Joback Method
dvisc	0.0008421	Pa×s	429.91	Joback Method
dvisc	0.0004011	Pa×s	474.17	Joback Method
dvisc	0.0002168	Pa×s	518.43	Joback Method
dvisc	0.0001291	Pa×s	562.69	Joback Method
dvisc	0.0000829	Pa×s	606.95	Joback Method
dvisc	0.0000566	Pa×s	651.21	Joback Method
hfust	2.93	kJ/mol	432.20	NIST Webbook
hfust	18.83	kJ/mol	420.70	NIST Webbook
psub	1.64e-03	kPa	377.80	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	0.06	kPa	417.30	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	0.06	kPa	417.30	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	0.05	kPa	415.40	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study

psub	0.04	kPa	411.40	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	0.02	kPa	406.40	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	0.02	kPa	401.30	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	0.01	kPa	399.30	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	9.73e-03	kPa	396.20	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	5.86e-03	kPa	391.00	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	2.85e-03	kPa	383.40	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
sfust	44.80	J/mol×K	420.70	NIST Webbook
sfust	6.78	J/mol×K	432.20	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Experimental standard molar enthalpies of formation of some 4-alkoxybenzoic acids:	https://www.doi.org/10.1016/j.jct.2009.08.007
Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study:	https://www.doi.org/10.1016/j.tca.2015.07.011
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=C1498960&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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
psub:	Sublimation pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume