Benzoic acid, 4-ethoxy-

Other names:	4-ethoxybenzoic acid
	Benzoic acid, p-ethoxy-
	p-ethoxybenzoic acid
	para-Ethoxybenzoic acid
Inchi:	InChI=1S/C9H10O3/c1-2-12-8-5-3-7(4-6-8)9(10)11/h3-6H,2H2,1H3,(H,10,11)
InchiKey:	SHSGDXCJYVZFTP-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	CCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	166.17
CAS:	619-86-3

Physical Properties

Property code	Value	Unit	Source
gf	-243.06	kJ/mol	Joback Method
hf	-401.06	kJ/mol	Joback Method
hfus	35.07	kJ/mol	Thermodynamic Study of 4-n-Alkyloxybenzoic Acids
hsub	123.30 ± 0.90	kJ/mol	NIST Webbook
hvap	64.40	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.783		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	605.45	K	Joback Method
tc	807.67	K	Joback Method
tf	472.80 ± 0.50	K	NIST Webbook
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.01	J/mol×K	605.45	Joback Method
cpg	313.16	J/mol×K	639.15	Joback Method
cpg	322.74	J/mol×K	672.86	Joback Method

cpg	331.76	J/mol×K	706.56	Joback Method
cpg	340.24	J/mol×K	740.27	Joback Method
cpg	348.17	J/mol×K	773.97	Joback Method
cpg	355.59	J/mol×K	807.67	Joback Method
dvisc	0.0011315	Pa×s	403.50	Joback Method
dvisc	0.0027550	Pa×s	363.11	Joback Method
dvisc	0.0005464	Pa×s	443.89	Joback Method
dvisc	0.0002980	Pa×s	484.28	Joback Method
dvisc	0.0001784	Pa×s	524.67	Joback Method
dvisc	0.0001149	Pa×s	565.06	Joback Method
dvisc	0.0000785	Pa×s	605.45	Joback Method
hfust	29.40	kJ/mol	472.80	NIST Webbook
hfust	29.40	kJ/mol	472.80	NIST Webbook

Sources

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 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=C619863&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
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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume