Benzoic acid, 4-ethoxy-, ethyl ester

Other names:	Benzoic acid, p-ethoxy-, ethyl ester
	Ethyl 4-ethoxybenzoate
	Ethyl para-ethoxybenzoate
	Ethyl p-ethoxybenzoate
	Benzoic acid, 4-ethyloxy-, ethyl ester
Inchi:	InChI=1S/C11H14O3/c1-3-13-10-7-5-9(6-8-10)11(12)14-4-2/h5-8H,3-4H2,1-2H3
InchiKey:	HRAQMGWTPNOILP-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCOC(=O)c1ccc(OCC)cc1
Mol. weight [g/mol]:	194.23
CAS:	23676-09-7

Physical Properties

Property code	Value	Unit	Source
gf	-194.40	kJ/mol	Joback Method
hf	-422.33	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	54.58	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.262		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1537.00		NIST Webbook
ripol	2593.00		NIST Webbook
ripol	2593.00		NIST Webbook
tb	548.20	K	NIST Webbook
tc	789.55	K	Joback Method
tf	347.06	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.80	J/mol×K	581.45	Joback Method
cpg	384.70	J/mol×K	616.13	Joback Method
cpg	397.90	J/mol×K	650.82	Joback Method
cpg	410.38	J/mol×K	685.50	Joback Method
cpg	422.16	J/mol×K	720.18	Joback Method
cpg	433.22	J/mol×K	754.87	Joback Method
cpg	443.58	J/mol×K	789.55	Joback Method
dvisc	0.0013141	Pa×s	347.06	Joback Method
dvisc	0.0007734	Pa×s	386.12	Joback Method
dvisc	0.0005017	Pa×s	425.19	Joback Method
dvisc	0.0003501	Pa×s	464.25	Joback Method
dvisc	0.0002583	Pa×s	503.32	Joback Method
dvisc	0.0001991	Pa×s	542.38	Joback Method
dvisc	0.0001589	Pa×s	581.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.70	K	1.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23676097&Units=SI

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

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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume