

Benzoic acid, 3-ethyloxy-, ethyl ester

Inchi:	InChI=1S/C11H14O3/c1-3-13-10-7-5-6-9(8-10)11(12)14-4-2/h5-8H,3-4H2,1-2H3
InchiKey:	BQXRZUDSLFBQDX-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCOC(=O)c1cccc(OCC)c1
Mol. weight [g/mol]:	194.23

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	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
tb	581.45	K	Joback Method
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

Sources

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=U374553&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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