

Carbonic acid, ethyl phenyl ester

Other names:	Ethyl phenyl carbonate Phenyl ethyl carbonate
Inchi:	InChI=1S/C9H10O3/c1-2-11-9(10)12-8-6-4-3-5-7-8/h3-7H,2H2,1H3
InchiKey:	YCNSGSUGQPDYTK-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	CCOC(=O)Oc1ccccc1
Mol. weight [g/mol]:	166.17
CAS:	3878-46-4

Physical Properties

Property code	Value	Unit	Source
gf	-201.61	kJ/mol	Joback Method
hf	-369.58	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	49.47	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.222		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
tb	530.71	K	Joback Method
tc	744.61	K	Joback Method
tf	312.00	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.36	J/mol×K	530.71	Joback Method
cpg	334.79	J/mol×K	708.96	Joback Method
cpg	324.98	J/mol×K	673.31	Joback Method
cpg	314.53	J/mol×K	637.66	Joback Method
cpg	303.45	J/mol×K	602.01	Joback Method

cpg	291.72	J/mol×K	566.36	Joback Method
cpg	343.96	J/mol×K	744.61	Joback Method
dvisc	0.0001920	Pa×s	530.71	Joback Method
dvisc	0.0002425	Pa×s	494.26	Joback Method
dvisc	0.0003179	Pa×s	457.81	Joback Method
dvisc	0.0004369	Pa×s	421.36	Joback Method
dvisc	0.0006375	Pa×s	384.90	Joback Method
dvisc	0.0010069	Pa×s	348.45	Joback Method
dvisc	0.0017696	Pa×s	312.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3878464&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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