

Carbonic acid, isobutyl phenyl ester

Other names:	Isobutyl phenyl carbonate Phenol, isoBOC
Inchi:	InChI=1S/C11H14O3/c1-9(2)8-13-11(12)14-10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3
InchiKey:	MTFSSQVLWRFNAZ-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CC(C)COC(=O)Oc1ccccc1
Mol. weight [g/mol]:	194.23
CAS:	13183-18-1

Physical Properties

Property code	Value	Unit	Source
gf	-187.21	kJ/mol	Joback Method
hf	-416.14	kJ/mol	Joback Method
hfus	18.74	kJ/mol	Joback Method
hvap	53.53	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.858		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1388.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1388.00		NIST Webbook
tb	576.03	K	Joback Method
tc	787.48	K	Joback Method
tf	319.54	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.61	J/molxK	576.03	Joback Method
cpg	386.12	J/molxK	611.27	Joback Method
cpg	399.83	J/molxK	646.51	Joback Method

cpg	412.76	J/molxK	681.76	Joback Method
cpg	424.90	J/molxK	717.00	Joback Method
cpg	436.27	J/molxK	752.24	Joback Method
cpg	446.86	J/molxK	787.48	Joback Method
dvisc	0.0021712	Paxs	319.54	Joback Method
dvisc	0.0010734	Paxs	362.29	Joback Method
dvisc	0.0006157	Paxs	405.04	Joback Method
dvisc	0.0003927	Paxs	447.78	Joback Method
dvisc	0.0002709	Paxs	490.53	Joback Method
dvisc	0.0001984	Paxs	533.28	Joback Method
dvisc	0.0001521	Paxs	576.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C13183181&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
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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