

Carbonic acid, 3-chlorophenyl isobutyl ester

Other names:	3-Chlorophenol, isoBOC
Inchi:	InChI=1S/C11H13ClO3/c1-8(2)7-14-11(13)15-10-5-3-4-9(12)6-10/h3-6,8H,7H2,1-2H3
InchiKey:	RHVHALPDQOPUPP-UHFFFAOYSA-N
Formula:	C11H13ClO3
SMILES:	CC(C)COC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	228.67

Physical Properties

Property code	Value	Unit	Source
gf	-208.77	kJ/mol	Joback Method
hf	-443.35	kJ/mol	Joback Method
hfus	22.55	kJ/mol	Joback Method
hvap	58.58	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.511		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1546.00		NIST Webbook
tb	618.44	K	Joback Method
tc	834.71	K	Joback Method
tf	361.98	K	Joback Method
vc	0.628	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.65	J/mol×K	618.44	Joback Method
cpg	411.04	J/mol×K	654.48	Joback Method
cpg	423.66	J/mol×K	690.53	Joback Method
cpg	435.49	J/mol×K	726.57	Joback Method
cpg	446.54	J/mol×K	762.62	Joback Method
cpg	456.82	J/mol×K	798.66	Joback Method
cpg	466.32	J/mol×K	834.71	Joback Method
dvisc	0.0014480	Paxs	361.98	Joback Method

dvisc	0.0008014	Paxs	404.72	Joback Method
dvisc	0.0004966	Paxs	447.47	Joback Method
dvisc	0.0003345	Paxs	490.21	Joback Method
dvisc	0.0002400	Paxs	532.95	Joback Method
dvisc	0.0001810	Paxs	575.70	Joback Method
dvisc	0.0001419	Paxs	618.44	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=U325645&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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