Carbonic acid, isobutyl 4-chlorophenyl ester

Other names: 4-Chlorophenol, isoBOC
Inchi: InChI=1S/C11H13ClO3/c1-8(2)7-14-11(13)15-10-5-3-9(12)4-6-10/h3-6,8H,7H2,1-2H3
InchiKey: SEKFJAYSWQQDNE-UHFFFAOYSA-N
Formula: C11H13ClO3
SMILES: CC(C)COC(=O)Oc1ccc(Cl)cc1
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	1565.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	618.44	K	Joback Method
tc	834.71	K	Joback Method
tf	361.98	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	466.32	J/mol×K	834.71	Joback Method
dvisc	0.0001419	Pa×s	618.44	Joback Method
dvisc	0.0001810	Pa×s	575.70	Joback Method
dvisc	0.0002400	Pa×s	532.95	Joback Method
dvisc	0.0003345	Pa×s	490.21	Joback Method
dvisc	0.0004966	Pa×s	447.47	Joback Method
dvisc	0.0008014	Pa×s	404.72	Joback Method
dvisc	0.0014480	Pa×s	361.98	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=U357832&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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