Isobutyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, isobutyl ester
Inchi: InChI=1S/C11H13ClO2/c1-8(2)7-14-11(13)9-4-3-5-10(12)6-9/h3-6,8H,7H2,1-2H3
InchiKey: DLJDIYXFPGOEBR-UHFFFAOYSA-N
Formula: C11H13ClO2
SMILES: CC(C)COC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 212.67

Physical Properties

Property code	Value	Unit	Source
gf	-103.77	kJ/mol	Joback Method
hf	-311.13	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.153		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1466.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	2004.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1969.00		NIST Webbook
tb	596.02	K	Joback Method
tc	814.94	K	Joback Method
tf	339.75	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.26	J/mol×K	596.02	Joback Method
cpg	386.90	J/mol×K	632.51	Joback Method
cpg	399.73	J/mol×K	668.99	Joback Method
cpg	411.74	J/mol×K	705.48	Joback Method
cpg	422.97	J/mol×K	741.97	Joback Method
cpg	433.43	J/mol×K	778.45	Joback Method
cpg	443.15	J/mol×K	814.94	Joback Method
dvisc	0.0019955	Pa×s	339.75	Joback Method
dvisc	0.0010666	Pa×s	382.46	Joback Method
dvisc	0.0006465	Pa×s	425.17	Joback Method
dvisc	0.0004294	Pa×s	467.88	Joback Method
dvisc	0.0003054	Pa×s	510.60	Joback Method
dvisc	0.0002290	Pa×s	553.31	Joback Method
dvisc	0.0001789	Pa×s	596.02	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373538&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume