sec-Butyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, 1-methylpropyl ester
Inchi: InChI=1S/C11H13ClO2/c1-3-8(2)14-11(13)9-5-4-6-10(12)7-9/h4-8H,3H2,1-2H3
InchiKey: OHLQBFGJSFFDLL-UHFFFAOYSA-N
Formula: C11H13ClO2
SMILES: CCC(C)OC(=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	-3.77		Crippen Method
logp	3.295		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1449.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1465.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1936.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1935.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1936.00		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	433.43	J/mol×K	778.45	Joback Method
cpg	422.97	J/mol×K	741.97	Joback Method
cpg	411.74	J/mol×K	705.48	Joback Method
cpg	399.73	J/mol×K	668.99	Joback Method
cpg	386.90	J/mol×K	632.51	Joback Method
cpg	443.15	J/mol×K	814.94	Joback Method
dvisc	0.0001789	Pa×s	596.02	Joback Method
dvisc	0.0002290	Pa×s	553.31	Joback Method
dvisc	0.0003054	Pa×s	510.60	Joback Method
dvisc	0.0004294	Pa×s	467.88	Joback Method
dvisc	0.0006465	Pa×s	425.17	Joback Method
dvisc	0.0010666	Pa×s	382.46	Joback Method
dvisc	0.0019955	Pa×s	339.75	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=U373551&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume