

Butyl 3-chlorobenzoate

Other names:	Benzoic acid, 3-chloro, butyl ester
Inchi:	InChI=1S/C11H13ClO2/c1-2-3-7-14-11(13)9-5-4-6-10(12)8-9/h4-6,8H,2-3,7H2,1H3
InchiKey:	UEGSDZZPMLTPSY-UHFFFAOYSA-N
Formula:	C11H13ClO2
SMILES:	CCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	212.67

Physical Properties

Property code	Value	Unit	Source
gf	-101.33	kJ/mol	Joback Method
hf	-305.85	kJ/mol	Joback Method
hfus	24.88	kJ/mol	Joback Method
hvap	56.56	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.297		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1549.00		NIST Webbook
rinpol	1517.00		NIST Webbook
ripol	2057.00		NIST Webbook
ripol	2056.00		NIST Webbook
tb	596.46	K	Joback Method
tc	810.87	K	Joback Method
tf	354.75	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.82	J/molxK	596.46	Joback Method
cpg	386.14	J/molxK	632.19	Joback Method
cpg	398.67	J/molxK	667.93	Joback Method
cpg	410.44	J/molxK	703.66	Joback Method
cpg	421.46	J/molxK	739.40	Joback Method

cpg	431.76	J/molxK	775.13	Joback Method
cpg	441.35	J/molxK	810.87	Joback Method
dvisc	0.0016178	Paxs	354.75	Joback Method
dvisc	0.0009457	Paxs	395.04	Joback Method
dvisc	0.0006105	Paxs	435.32	Joback Method
dvisc	0.0004245	Paxs	475.61	Joback Method
dvisc	0.0003124	Paxs	515.89	Joback Method
dvisc	0.0002403	Paxs	556.17	Joback Method
dvisc	0.0001915	Paxs	596.46	Joback Method

Sources

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=U373552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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