Benzoic acid, 2-chloro, butyl ester

Inchi: InChI=1S/C11H13ClO2/c1-2-3-8-14-11(13)9-6-4-5-7-10(9)12/h4-7H,2-3,8H2,1H3
InchiKey: YOAQWDULOOZKPL-UHFFFAOYSA-N
Formula: C11H13ClO2
SMILES: CCCCOC(=O)c1ccccc1Cl
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	1540.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1529.00		NIST Webbook
ripol	2144.00		NIST Webbook
ripol	2184.00		NIST Webbook
ripol	2147.00		NIST Webbook
ripol	2108.00		NIST Webbook
ripol	2126.00		NIST Webbook
ripol	2153.00		NIST Webbook
ripol	2144.00		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/mol×K	596.46	Joback Method
cpg	386.14	J/mol×K	632.19	Joback Method
cpg	398.67	J/mol×K	667.93	Joback Method
cpg	410.44	J/mol×K	703.66	Joback Method
cpg	421.46	J/mol×K	739.40	Joback Method
cpg	431.76	J/mol×K	775.13	Joback Method
cpg	441.35	J/mol×K	810.87	Joback Method
dvisc	0.0016178	Pa×s	354.75	Joback Method
dvisc	0.0009457	Pa×s	395.04	Joback Method
dvisc	0.0006105	Pa×s	435.32	Joback Method
dvisc	0.0004245	Pa×s	475.61	Joback Method
dvisc	0.0003124	Pa×s	515.89	Joback Method
dvisc	0.0002403	Pa×s	556.17	Joback Method
dvisc	0.0001915	Pa×s	596.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R31355&Units=SI
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

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