4-Butylbenzoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C17H17ClO2/c1-2-3-4-13-5-7-14(8-6-13)17(19)20-16-11-9-15(18)10-12-16/h5-
InchiKey: KFSDSHJKHABQJV-UHFFFAOYSA-N
Formula: C17H17ClO2
SMILES: CCCCc1ccc(C(=O)Oc2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 288.77

Physical Properties

Property code	Value	Unit	Source
gf	51.97	kJ/mol	Joback Method
hf	-204.63	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.902		Crippen Method
mcvol	222.550	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	2268.00		NIST Webbook
rinpol	2268.00		NIST Webbook
tb	765.40	K	Joback Method
tc	998.16	K	Joback Method
tf	461.31	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.38	J/mol×K	765.40	Joback Method
cpg	611.18	J/mol×K	804.19	Joback Method
cpg	624.81	J/mol×K	842.99	Joback Method
cpg	637.32	J/mol×K	881.78	Joback Method
cpg	648.76	J/mol×K	920.57	Joback Method
cpg	659.17	J/mol×K	959.37	Joback Method
cpg	668.61	J/mol×K	998.16	Joback Method
dvisc	0.0007967	Pa×s	461.31	Joback Method

dvisc	0.0004745	Pa×s	511.99	Joback Method
dvisc	0.0003102	Pa×s	562.67	Joback Method
dvisc	0.0002176	Pa×s	613.36	Joback Method
dvisc	0.0001611	Pa×s	664.04	Joback Method
dvisc	0.0001245	Pa×s	714.72	Joback Method
dvisc	0.0000995	Pa×s	765.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307504&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume