4-Butylbenzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C17H16Cl2O2/c1-2-3-4-12-5-7-13(8-6-12)17(20)21-14-9-10-15(18)16(19)11-14
InchiKey: CJIWMGIVONTUCE-UHFFFAOYSA-N
Formula: C17H16Cl2O2
SMILES: CCCCc1ccc(C(=O)Oc2ccc(Cl)c(Cl)c2)cc1
Mol. weight [g/mol]: 323.21

Physical Properties

Property code	Value	Unit	Source
gf	30.41	kJ/mol	Joback Method
hf	-231.84	kJ/mol	Joback Method
hfus	37.88	kJ/mol	Joback Method
hvap	77.90	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.555		Crippen Method
mcvol	234.790	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	2473.00		NIST Webbook
rinpol	2473.00		NIST Webbook
tb	807.81	K	Joback Method
tc	1043.74	K	Joback Method
tf	503.75	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.17	J/mol×K	807.81	Joback Method
cpg	632.55	J/mol×K	847.13	Joback Method
cpg	644.80	J/mol×K	886.45	Joback Method
cpg	655.97	J/mol×K	925.77	Joback Method
cpg	666.10	J/mol×K	965.10	Joback Method
cpg	675.24	J/mol×K	1004.42	Joback Method
cpg	683.43	J/mol×K	1043.74	Joback Method
dvisc	0.0005961	Pa×s	503.75	Joback Method

dvisc	0.0003763	Pa×s	554.43	Joback Method
dvisc	0.0002566	Pa×s	605.10	Joback Method
dvisc	0.0001856	Pa×s	655.78	Joback Method
dvisc	0.0001407	Pa×s	706.46	Joback Method
dvisc	0.0001106	Pa×s	757.13	Joback Method
dvisc	0.0000897	Pa×s	807.81	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=U307508&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume