4-Butylbenzoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C17H14Cl4O2/c1-2-3-4-10-5-7-11(8-6-10)17(22)23-16-13(19)9-12(18)14(20)15

InchiKey: VJFPTLHFDFYZGH-UHFFFAOYSA-N

Formula: C17H14Cl4O2

SMILES: CCCCc1ccc(C(=O)Oc2c(Cl)cc(Cl)c(Cl)c2Cl)cc1

Mol. weight [g/mol]: 392.10

Physical Properties

Property code	Value	Unit	Source
gf	-12.71	kJ/mol	Joback Method
hf	-286.26	kJ/mol	Joback Method
hfus	45.50	kJ/mol	Joback Method
hvap	87.99	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.862		Crippen Method
mcvol	259.270	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2809.00		NIST Webbook
rinpol	2809.00		NIST Webbook
tb	892.63	K	Joback Method
tc	1134.80	K	Joback Method
tf	588.63	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.63	J/mol×K	892.63	Joback Method
cpg	701.73	J/mol×K	1094.43	Joback Method
cpg	695.11	J/mol×K	1054.07	Joback Method
cpg	687.53	J/mol×K	1013.71	Joback Method
cpg	678.94	J/mol×K	973.35	Joback Method
cpg	669.32	J/mol×K	932.99	Joback Method
cpg	707.41	J/mol×K	1134.80	Joback Method
dvisc	0.0000708	Pa×s	892.63	Joback Method

dvisc	0.0000854	Pa×s	841.96	Joback Method
dvisc	0.0001055	Pa×s	791.30	Joback Method
dvisc	0.0001340	Pa×s	740.63	Joback Method
dvisc	0.0001765	Pa×s	689.96	Joback Method
dvisc	0.0002428	Pa×s	639.30	Joback Method
dvisc	0.0003528	Pa×s	588.63	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=U354324&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume