4-Butylbenzoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C17H15Cl3O2/c1-2-3-4-11-5-7-12(8-6-11)17(21)22-16-10-14(19)13(18)9-15(16

InchiKey: KBTMBSDYUZPJLZ-UHFFFAOYSA-N

Formula: C17H15Cl3O2

SMILES: CCCCc1ccc(C(=O)Oc2cc(Cl)c(Cl)cc2Cl)cc1

Mol. weight [g/mol]: 357.66

Physical Properties

Property code	Value	Unit	Source
gf	8.85	kJ/mol	Joback Method
hf	-259.05	kJ/mol	Joback Method
hfus	41.69	kJ/mol	Joback Method
hvap	82.95	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.209		Crippen Method
mcvol	247.030	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	2692.00		NIST Webbook
tb	850.22	K	Joback Method
tc	1089.25	K	Joback Method
tf	546.19	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.88	J/mol×K	850.22	Joback Method
cpg	651.89	J/mol×K	890.06	Joback Method
cpg	662.81	J/mol×K	929.90	Joback Method
cpg	672.68	J/mol×K	969.74	Joback Method
cpg	681.53	J/mol×K	1009.57	Joback Method
cpg	689.41	J/mol×K	1049.41	Joback Method
cpg	696.35	J/mol×K	1089.25	Joback Method
dvisc	0.0004551	Pa×s	546.19	Joback Method
dvisc	0.0003012	Pa×s	596.86	Joback Method

dvisc	0.0002126	Pa×s	647.53	Joback Method
dvisc	0.0001579	Pa×s	698.21	Joback Method
dvisc	0.0001221	Pa×s	748.88	Joback Method
dvisc	0.0000975	Pa×s	799.55	Joback Method
dvisc	0.0000800	Pa×s	850.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354323&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