4-Butylbenzoic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C13H15Cl3O2/c1-2-3-4-10-5-7-11(8-6-10)12(17)18-9-13(14,15)16/h5-8H,2-4,9
InchiKey: NPEJHXJLBOHWPV-UHFFFAOYSA-N
Formula: C13H15Cl3O2
SMILES: CCCCc1ccc(C(=O)OCC(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]: 309.62

Physical Properties

Property code	Value	Unit	Source
gf	-105.51	kJ/mol	Joback Method
hf	-387.36	kJ/mol	Joback Method
hfus	31.04	kJ/mol	Joback Method
hvap	68.48	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.556		Crippen Method
mcvol	214.430	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	713.85	K	Joback Method
tc	939.31	K	Joback Method
tf	439.55	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.87	J/mol×K	713.85	Joback Method
cpg	581.23	J/mol×K	901.73	Joback Method
cpg	571.89	J/mol×K	864.16	Joback Method
cpg	561.74	J/mol×K	826.58	Joback Method
cpg	550.72	J/mol×K	789.00	Joback Method
cpg	538.79	J/mol×K	751.43	Joback Method
cpg	589.82	J/mol×K	939.31	Joback Method
dvisc	0.0001074	Pa×s	713.85	Joback Method

dvisc	0.0001383	Pa×s	668.13	Joback Method
dvisc	0.0001848	Pa×s	622.42	Joback Method
dvisc	0.0002587	Pa×s	576.70	Joback Method
dvisc	0.0003837	Pa×s	530.98	Joback Method
dvisc	0.0006128	Pa×s	485.27	Joback Method
dvisc	0.0010790	Pa×s	439.55	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=U354319&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