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

Inchi: InChI=1S/C13H6Cl4O2/c14-8-6-9(15)12(11(17)10(8)16)19-13(18)7-4-2-1-3-5-7/h1-6H
InchiKey: XCOILKOWUZFKKG-UHFFFAOYSA-N
Formula: C13H6Cl4O2
SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1ccccc1
Mol. weight [g/mol]: 336.00

Physical Properties

Property code	Value	Unit	Source
gf	-36.76	kJ/mol	Joback Method
hf	-192.23	kJ/mol	Joback Method
hfus	35.53	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.519		Crippen Method
mcvol	202.910	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
tb	796.13	K	Joback Method
tc	1055.94	K	Joback Method
tf	531.03	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.65	J/mol×K	796.13	Joback Method
cpg	455.79	J/mol×K	839.43	Joback Method
cpg	463.95	J/mol×K	882.73	Joback Method
cpg	471.17	J/mol×K	926.03	Joback Method
cpg	477.47	J/mol×K	969.33	Joback Method
cpg	482.89	J/mol×K	1012.64	Joback Method
cpg	487.47	J/mol×K	1055.94	Joback Method
dvisc	0.0005512	Pa×s	531.03	Joback Method

dvisc	0.0003867	Pa×s	575.21	Joback Method
dvisc	0.0002854	Pa×s	619.40	Joback Method
dvisc	0.0002193	Pa×s	663.58	Joback Method
dvisc	0.0001742	Pa×s	707.76	Joback Method
dvisc	0.0001421	Pa×s	751.95	Joback Method
dvisc	0.0001186	Pa×s	796.13	Joback Method

Sources

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=U360687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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