Benzoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C13H7Cl3O2/c14-9-6-11(16)12(7-10(9)15)18-13(17)8-4-2-1-3-5-8/h1-7H
InchiKey: MDWSVFVNPWZKMU-UHFFFAOYSA-N
Formula: C13H7Cl3O2
SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccccc1
Mol. weight [g/mol]: 301.55

Physical Properties

Property code	Value	Unit	Source
gf	-15.20	kJ/mol	Joback Method
hf	-165.02	kJ/mol	Joback Method
hfus	31.72	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.866		Crippen Method
mcvol	190.670	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	753.72	K	Joback Method
tc	1011.22	K	Joback Method
tf	488.59	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.57	J/mol×K	753.72	Joback Method
cpg	471.87	J/mol×K	968.30	Joback Method
cpg	465.30	J/mol×K	925.39	Joback Method
cpg	457.83	J/mol×K	882.47	Joback Method
cpg	449.40	J/mol×K	839.55	Joback Method
cpg	440.00	J/mol×K	796.64	Joback Method
cpg	477.58	J/mol×K	1011.22	Joback Method
dvisc	0.0001318	Pa×s	753.72	Joback Method

dvisc	0.0001598	Pa×s	709.53	Joback Method
dvisc	0.0001988	Pa×s	665.34	Joback Method
dvisc	0.0002550	Pa×s	621.15	Joback Method
dvisc	0.0003399	Pa×s	576.97	Joback Method
dvisc	0.0004751	Pa×s	532.78	Joback Method
dvisc	0.0007055	Pa×s	488.59	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=U360686&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