

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

Inchi:	InChI=1S/C13H6Cl4O2/c14-8-4-2-1-3-7(8)13(18)19-12-6-10(16)9(15)5-11(12)17/h1-6H
InchiKey:	WJBRLTCUKHJWLX-UHFFFAOYSA-N
Formula:	C13H6Cl4O2
SMILES:	O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccccc1Cl
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
rinpola	2399.00		NIST Webbook
tb	796.13	K	Joback Method
tc	1055.94	K	Joback Method
tf	531.03	K	Joback Method
vc	0.767	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.65	J/molxK	796.13	Joback Method
cpg	455.79	J/molxK	839.43	Joback Method
cpg	463.95	J/molxK	882.73	Joback Method
cpg	471.17	J/molxK	926.03	Joback Method
cpg	477.47	J/molxK	969.33	Joback Method
cpg	482.89	J/molxK	1012.64	Joback Method
cpg	487.47	J/molxK	1055.94	Joback Method
dvisc	0.0005512	Paxs	531.03	Joback Method
dvisc	0.0003867	Paxs	575.21	Joback Method

dvisc	0.0002854	Paxs	619.40	Joback Method
dvisc	0.0002193	Paxs	663.58	Joback Method
dvisc	0.0001742	Paxs	707.76	Joback Method
dvisc	0.0001421	Paxs	751.95	Joback Method
dvisc	0.0001186	Paxs	796.13	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U360528&Units=SI

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

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