

3-Chlorobenzoic acid, 2,3-dichlorophenyl ester

Inchi: InChI=1S/C13H7Cl3O2/c14-9-4-1-3-8(7-9)13(17)18-11-6-2-5-10(15)12(11)16/h1-7H
InchiKey: DQRNBBSBPPHFSG-UHFFFAOYSA-N
Formula: C13H7Cl3O2
SMILES: O=C(Oc1cccc(Cl)c1Cl)c1cccc(Cl)c1
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
rinpola	2252.00		NIST Webbook
tb	753.72	K	Joback Method
tc	1011.22	K	Joback Method
tf	488.59	K	Joback Method
vc	0.719	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.57	J/molxK	753.72	Joback Method
cpg	471.87	J/molxK	968.30	Joback Method
cpg	465.30	J/molxK	925.39	Joback Method
cpg	457.83	J/molxK	882.47	Joback Method
cpg	449.40	J/molxK	839.55	Joback Method
cpg	440.00	J/molxK	796.64	Joback Method
cpg	477.58	J/molxK	1011.22	Joback Method
dvisc	0.0001318	Paxs	753.72	Joback Method
dvisc	0.0001598	Paxs	709.53	Joback Method

dvisc	0.0001988	Paxs	665.34	Joback Method
dvisc	0.0002550	Paxs	621.15	Joback Method
dvisc	0.0003399	Paxs	576.97	Joback Method
dvisc	0.0004751	Paxs	532.78	Joback Method
dvisc	0.0007055	Paxs	488.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357401&Units=SI
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

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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