3,4-Dichlorobenzoic acid, 4-isopropyl phenyl ester

Inchi: InChI=1S/C16H14Cl2O2/c1-10(2)11-3-6-13(7-4-11)20-16(19)12-5-8-14(17)15(18)9-12/h3

InchiKey: KUYPPVGCZIGLAH-UHFFFAOYSA-N

Formula: C16H14Cl2O2

SMILES: CC(C)c1ccc(OC(=O)c2ccc(Cl)c(Cl)c2)cc1

Mol. weight [g/mol]: 309.19

CAS: 116465-99-7

Physical Properties

Property code	Value	Unit	Source
gf	19.55	kJ/mol	Joback Method
hf	-216.48	kJ/mol	Joback Method
hfus	31.77	kJ/mol	Joback Method
hvap	75.29	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.336		Crippen Method
mcvol	220.700	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
tb	784.49	K	Joback Method
tc	1028.94	K	Joback Method
tf	477.48	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.55	J/mol×K	784.49	Joback Method
cpg	578.85	J/mol×K	825.23	Joback Method
cpg	590.99	J/mol×K	865.97	Joback Method
cpg	602.00	J/mol×K	906.72	Joback Method
cpg	611.93	J/mol×K	947.46	Joback Method
cpg	620.82	J/mol×K	988.20	Joback Method
cpg	628.72	J/mol×K	1028.94	Joback Method
dvisc	0.0007133	Pa×s	477.48	Joback Method
dvisc	0.0004316	Pa×s	528.65	Joback Method

dvisc	0.0002853	Pa×s	579.82	Joback Method
dvisc	0.0002017	Pa×s	630.99	Joback Method
dvisc	0.0001502	Pa×s	682.15	Joback Method
dvisc	0.0001166	Pa×s	733.32	Joback Method
dvisc	0.0000935	Pa×s	784.49	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=C116465997&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume