

3,4-Dichlorobenzoic acid, 4-sec-butylphenyl ester

Inchi:	InChI=1S/C17H16Cl2O2/c1-3-11(2)12-4-7-14(8-5-12)21-17(20)13-6-9-15(18)16(19)10-1
InchiKey:	LLWWZWKTVYXRGI-UHFFFAOYSA-N
Formula:	C17H16Cl2O2
SMILES:	CCC(C)c1ccc(OC(=O)c2ccc(Cl)c(Cl)c2)cc1
Mol. weight [g/mol]:	323.21
CAS:	109157-31-5

Physical Properties

Property code	Value	Unit	Source
gf	27.97	kJ/mol	Joback Method
hf	-237.12	kJ/mol	Joback Method
hfus	34.36	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.726		Crippen Method
mcvol	234.790	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
tb	807.37	K	Joback Method
tc	1047.33	K	Joback Method
tf	488.75	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.76	J/molxK	807.37	Joback Method
cpg	633.36	J/molxK	847.36	Joback Method
cpg	645.77	J/molxK	887.36	Joback Method
cpg	657.06	J/molxK	927.35	Joback Method
cpg	667.25	J/molxK	967.35	Joback Method
cpg	676.41	J/molxK	1007.34	Joback Method
cpg	684.57	J/molxK	1047.33	Joback Method
dvisc	0.0006573	Paxs	488.75	Joback Method
dvisc	0.0003924	Paxs	541.85	Joback Method

dvisc	0.0002568	Paxs	594.96	Joback Method
dvisc	0.0001802	Paxs	648.06	Joback Method
dvisc	0.0001334	Paxs	701.16	Joback Method
dvisc	0.0001030	Paxs	754.27	Joback Method
dvisc	0.0000823	Paxs	807.37	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=C109157315&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

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