

2,4-Dichlorobenzoic acid, 2,4-dimethyl phenyl ester

Inchi:	InChI=1S/C15H12Cl2O2/c1-9-3-6-14(10(2)7-9)19-15(18)12-5-4-11(16)8-13(12)17/h3-8H
InchiKey:	ILGOUYRLPKQKPE-UHFFFAOYSA-N
Formula:	C15H12Cl2O2
SMILES:	<chem>Cc1ccc(OC(=O)c2ccc(Cl)cc2Cl)c(C)c1</chem>
Mol. weight [g/mol]:	295.16
CAS:	116465-98-6

Physical Properties

Property code	Value	Unit	Source
gf	3.94	kJ/mol	Joback Method
hf	-202.03	kJ/mol	Joback Method
hfus	32.31	kJ/mol	Joback Method
hvap	74.11	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.829		Crippen Method
mcvol	206.610	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
tb	767.03	K	Joback Method
tc	1012.56	K	Joback Method
tf	493.73	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.29	J/molxK	767.03	Joback Method
cpg	522.87	J/molxK	807.95	Joback Method
cpg	534.37	J/molxK	848.87	Joback Method
cpg	544.83	J/molxK	889.80	Joback Method
cpg	554.28	J/molxK	930.72	Joback Method
cpg	562.74	J/molxK	971.64	Joback Method
cpg	570.24	J/molxK	1012.56	Joback Method
dvisc	0.0006070	Paxs	493.73	Joback Method
dvisc	0.0004098	Paxs	539.28	Joback Method

dvisc	0.0002942	Paxs	584.83	Joback Method
dvisc	0.0002215	Paxs	630.38	Joback Method
dvisc	0.0001733	Paxs	675.93	Joback Method
dvisc	0.0001399	Paxs	721.48	Joback Method
dvisc	0.0001158	Paxs	767.03	Joback Method

Sources

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=C116465986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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