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: Cc1ccc(OC(=O)c2ccc(Cl)cc2Cl)c(C)c1
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/mol×K	767.03	Joback Method
cpg	522.87	J/mol×K	807.95	Joback Method
cpg	534.37	J/mol×K	848.87	Joback Method
cpg	544.83	J/mol×K	889.80	Joback Method
cpg	554.28	J/mol×K	930.72	Joback Method
cpg	562.74	J/mol×K	971.64	Joback Method
cpg	570.24	J/mol×K	1012.56	Joback Method
dvisc	0.0006070	Pa×s	493.73	Joback Method
dvisc	0.0004098	Pa×s	539.28	Joback Method

dvisc	0.0002942	Pa×s	584.83	Joback Method
dvisc	0.0002215	Pa×s	630.38	Joback Method
dvisc	0.0001733	Pa×s	675.93	Joback Method
dvisc	0.0001399	Pa×s	721.48	Joback Method
dvisc	0.0001158	Pa×s	767.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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