

2-Hydroxybenzoic acid, 2,4-dichlorophenyl ester

Inchi:	InChI=1S/C13H8Cl2O3/c14-8-5-6-12(10(15)7-8)18-13(17)9-3-1-2-4-11(9)16/h1-7,16H
InchiKey:	QHZASEYQTUBNIA-UHFFFAOYSA-N
Formula:	C13H8Cl2O3
SMILES:	O=C(Oc1ccc(Cl)cc1Cl)c1ccccc1O
Mol. weight [g/mol]:	283.11
CAS:	2944-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-148.26	kJ/mol	Joback Method
hf	-315.12	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	81.35	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.918		Crippen Method
mcvol	184.300	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	791.93	K	Joback Method
tc	1052.55	K	Joback Method
tf	557.87	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.94	J/molxK	791.93	Joback Method
cpg	494.96	J/molxK	1009.11	Joback Method
cpg	487.19	J/molxK	965.68	Joback Method
cpg	479.02	J/molxK	922.24	Joback Method
cpg	470.33	J/molxK	878.80	Joback Method
cpg	461.01	J/molxK	835.37	Joback Method
cpg	502.44	J/molxK	1052.55	Joback Method
dvisc	0.0000089	Paxs	791.93	Joback Method
dvisc	0.0000122	Paxs	752.92	Joback Method

dvisc	0.0000172	Paxs	713.91	Joback Method
dvisc	0.0000251	Paxs	674.90	Joback Method
dvisc	0.0000386	Paxs	635.89	Joback Method
dvisc	0.0000628	Paxs	596.88	Joback Method
dvisc	0.0001091	Paxs	557.87	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=C2944594&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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