3-(3,4-DICHLOROPHENOXY)BENZALDEHYDE

Other names: Benzaldehyde, 3-(3,4-dichlorophenoxy)-
3-(3,4-Dichlorophenoxy)benzaldehyde
Inchi: InChI=1S/C13H8Cl2O2/c14-12-5-4-11(7-13(12)15)17-10-3-1-2-9(6-10)8-16/h1-8H
InchiKey: ABQHJSHFFLAGHF-UHFFFAOYSA-N
Formula: C13H8Cl2O2
SMILES: O=Cc1cccc(Oc2ccc(Cl)c(Cl)c2)c1
Mol. weight [g/mol]: 267.11

Physical Properties

Property code	Value	Unit	Source
hfus	28.21	kJ/mol	Joback Method
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-5.31		Cheméo Relay (1.0)
logp	4.598		Crippen Method
mcvol	178.430	ml/mol	McGowan Method
tb	620.69	K	Cheméo Relay (1.0)
tf	339.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.90	J/mol×K	711.08	Joback Method
cpg	421.30	J/mol×K	752.81	Joback Method
cpg	431.70	J/mol×K	794.54	Joback Method
cpg	441.15	J/mol×K	836.27	Joback Method
cpg	449.68	J/mol×K	878.00	Joback Method
cpg	457.32	J/mol×K	919.74	Joback Method
cpg	464.11	J/mol×K	961.47	Joback Method
dvisc	0.0008890	Pa×s	450.74	Joback Method
dvisc	0.0005900	Pa×s	494.13	Joback Method
dvisc	0.0004183	Pa×s	537.52	Joback Method
dvisc	0.0003122	Pa×s	580.91	Joback Method
dvisc	0.0002427	Pa×s	624.30	Joback Method
dvisc	0.0001950	Pa×s	667.69	Joback Method

dvisc	0.0001608	Pa×s	711.08	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79124768&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point