4-(1,1-Dimethylhexyl)phenyl 2,4-dichlorobenzoate

Inchi: InChI=1S/C21H24Cl2O2/c1-4-5-6-13-21(2,3)15-7-10-17(11-8-15)25-20(24)18-12-9-16(22

InchiKey: ZKGUILLUXMCPJA-UHFFFAOYSA-N

Formula: C21H24Cl2O2

SMILES: CCCCCC(C)(C)c1ccc(OC(=O)c2ccc(Cl)cc2Cl)cc1

Mol. weight [g/mol]: 379.32

Physical Properties

Property code	Value	Unit	Source
gf	66.93	kJ/mol	Joback Method
hf	-323.15	kJ/mol	Joback Method
hfus	40.83	kJ/mol	Joback Method
hvap	85.51	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	7.071		Crippen Method
mcvol	291.150	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
tb	896.10	K	Joback Method
tc	1129.53	K	Joback Method
tf	551.25	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.12	J/mol×K	896.10	Joback Method
cpg	860.55	J/mol×K	935.01	Joback Method
cpg	873.81	J/mol×K	973.91	Joback Method
cpg	885.99	J/mol×K	1012.82	Joback Method
cpg	897.17	J/mol×K	1051.72	Joback Method
cpg	907.43	J/mol×K	1090.63	Joback Method
cpg	916.87	J/mol×K	1129.53	Joback Method
dvisc	0.0003674	Pa×s	551.25	Joback Method
dvisc	0.0002141	Pa×s	608.73	Joback Method
dvisc	0.0001370	Pa×s	666.20	Joback Method

dvisc	0.0000941	Pa×s	723.67	Joback Method
dvisc	0.0000683	Pa×s	781.15	Joback Method
dvisc	0.0000518	Pa×s	838.62	Joback Method
dvisc	0.0000407	Pa×s	896.10	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=B6004133&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