3,3-Dimethylbutan-2-yl 3-chlorobenzoate

Inchi: InChI=1S/C13H17ClO2/c1-9(13(2,3)4)16-12(15)10-6-5-7-11(14)8-10/h5-9H,1-4H3
InchiKey: KUBCEMWGSNRTPX-UHFFFAOYSA-N
Formula: C13H17ClO2
SMILES: CC(OC(=O)c1cccc(Cl)c1)C(C)(C)C
Mol. weight [g/mol]: 240.73

Physical Properties

Property code	Value	Unit	Source
gf	-84.09	kJ/mol	Joback Method
hf	-361.16	kJ/mol	Joback Method
hfus	19.13	kJ/mol	Joback Method
hvap	59.33	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.931		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1598.00		NIST Webbook
tb	638.55	K	Joback Method
tc	862.36	K	Joback Method
tf	364.71	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.98	J/mol×K	638.55	Joback Method
cpg	542.75	J/mol×K	825.06	Joback Method
cpg	531.15	J/mol×K	787.76	Joback Method
cpg	518.62	J/mol×K	750.46	Joback Method
cpg	505.12	J/mol×K	713.15	Joback Method
cpg	490.59	J/mol×K	675.85	Joback Method
cpg	553.47	J/mol×K	862.36	Joback Method
dvisc	0.0001261	Pa×s	638.55	Joback Method
dvisc	0.0001671	Pa×s	592.91	Joback Method

dvisc	0.0002321	Pa×s	547.27	Joback Method
dvisc	0.0003422	Pa×s	501.63	Joback Method
dvisc	0.0005452	Pa×s	455.99	Joback Method
dvisc	0.0009635	Pa×s	410.35	Joback Method
dvisc	0.0019636	Pa×s	364.71	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=U373574&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume