4-Methylpentan-2-yl 3-chlorobenzoate

Inchi: InChI=1S/C13H17ClO2/c1-9(2)7-10(3)16-13(15)11-5-4-6-12(14)8-11/h4-6,8-10H,7H2,1-3
InchiKey: NODVZAWIUXDGOW-UHFFFAOYSA-N
Formula: C13H17ClO2
SMILES: CC(C)CC(C)OC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 240.73

Physical Properties

Property code	Value	Unit	Source
gf	-89.37	kJ/mol	Joback Method
hf	-357.69	kJ/mol	Joback Method
hfus	23.02	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.931		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1612.00		NIST Webbook
tb	641.34	K	Joback Method
tc	857.10	K	Joback Method
tf	347.29	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.31	J/mol×K	641.34	Joback Method
cpg	487.59	J/mol×K	677.30	Joback Method
cpg	501.92	J/mol×K	713.26	Joback Method
cpg	515.33	J/mol×K	749.22	Joback Method
cpg	527.84	J/mol×K	785.18	Joback Method
cpg	539.49	J/mol×K	821.14	Joback Method
cpg	550.28	J/mol×K	857.10	Joback Method
dvisc	0.0022528	Pa×s	347.29	Joback Method
dvisc	0.0010544	Pa×s	396.30	Joback Method

dvisc	0.0005833	Pa×s	445.31	Joback Method
dvisc	0.0003629	Pa×s	494.31	Joback Method
dvisc	0.0002459	Pa×s	543.32	Joback Method
dvisc	0.0001778	Pa×s	592.33	Joback Method
dvisc	0.0001350	Pa×s	641.34	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=U373575&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume