3-Methylpentan-3-yl 3-chlorobenzoate

Inchi: InChI=1S/C13H17ClO2/c1-4-13(3,5-2)16-12(15)10-7-6-8-11(14)9-10/h6-9H,4-5H2,1-3H3
InchiKey: SJNSMUALWJBEGP-UHFFFAOYSA-N
Formula: C13H17ClO2
SMILES: CCC(C)(CC)OC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 240.73

Physical Properties

Property code	Value	Unit	Source
gf	-81.65	kJ/mol	Joback Method
hf	-355.88	kJ/mol	Joback Method
hfus	22.65	kJ/mol	Joback Method
hvap	59.72	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.075		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
tb	638.99	K	Joback Method
tc	858.34	K	Joback Method
tf	379.71	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.50	J/mol×K	638.99	Joback Method
cpg	489.76	J/mol×K	675.55	Joback Method
cpg	504.00	J/mol×K	712.11	Joback Method
cpg	517.25	J/mol×K	748.67	Joback Method
cpg	529.58	J/mol×K	785.23	Joback Method
cpg	541.02	J/mol×K	821.78	Joback Method
cpg	551.63	J/mol×K	858.34	Joback Method
dvisc	0.0015782	Pa×s	379.71	Joback Method

dvisc	0.0008507	Pa×s	422.92	Joback Method
dvisc	0.0005142	Pa×s	466.14	Joback Method
dvisc	0.0003385	Pa×s	509.35	Joback Method
dvisc	0.0002379	Pa×s	552.56	Joback Method
dvisc	0.0001760	Pa×s	595.78	Joback Method
dvisc	0.0001356	Pa×s	638.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373571&Units=SI
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

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

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