

2-Chlorobenzoic acid, 2-methylpentyl ester

Inchi:	InChI=1S/C13H17ClO2/c1-3-6-10(2)9-16-13(15)11-7-4-5-8-12(11)14/h4-5,7-8,10H,3,6,9H
InchiKey:	POKLGWFGOJKHSV-UHFFFAOYSA-N
Formula:	C13H17ClO2
SMILES:	CCCC(C)COC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	240.73

Physical Properties

Property code	Value	Unit	Source
gf	-86.93	kJ/mol	Joback Method
hf	-352.41	kJ/mol	Joback Method
hfus	26.54	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.933		Crippen Method
mvol	189.950	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1724.00		NIST Webbook
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tb	641.78	K	Joback Method
tc	853.39	K	Joback Method
tf	362.29	K	Joback Method
vc	0.723	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.84	J/molxK	641.78	Joback Method
cpg	486.78	J/molxK	677.05	Joback Method
cpg	500.82	J/molxK	712.32	Joback Method
cpg	513.99	J/molxK	747.58	Joback Method
cpg	526.31	J/molxK	782.85	Joback Method
cpg	537.80	J/molxK	818.12	Joback Method
cpg	548.48	J/molxK	853.39	Joback Method
dvisc	0.0017997	Paxs	362.29	Joback Method

dvisc	0.0009315	Paxs	408.87	Joback Method
dvisc	0.0005517	Paxs	455.45	Joback Method
dvisc	0.0003601	Paxs	502.03	Joback Method
dvisc	0.0002527	Paxs	548.62	Joback Method
dvisc	0.0001874	Paxs	595.20	Joback Method
dvisc	0.0001452	Paxs	641.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360522&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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