2-Chlorobenzoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C13H17ClO3/c1-10(7-8-16-2)9-17-13(15)11-5-3-4-6-12(11)14/h3-6,10H,7-9H2

InchiKey: AOYQHRUPNZPJHW-UHFFFAOYSA-N

Formula: C13H17ClO3

SMILES: COCCC(C)COC(=O)c1ccccc1Cl

Mol. weight [g/mol]: 256.73

Physical Properties

Property code	Value	Unit	Source
gf	-191.93	kJ/mol	Joback Method
hf	-484.63	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	63.03	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.169		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
tb	664.20	K	Joback Method
tc	873.60	K	Joback Method
tf	384.52	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.88	J/mol×K	664.20	Joback Method
cpg	512.51	J/mol×K	699.10	Joback Method
cpg	526.26	J/mol×K	734.00	Joback Method
cpg	539.15	J/mol×K	768.90	Joback Method
cpg	551.19	J/mol×K	803.80	Joback Method
cpg	562.37	J/mol×K	838.70	Joback Method
cpg	572.71	J/mol×K	873.60	Joback Method
dvisc	0.0012831	Pa×s	384.52	Joback Method

dvisc	0.0006881	Pa×s	431.13	Joback Method
dvisc	0.0004167	Pa×s	477.75	Joback Method
dvisc	0.0002759	Pa×s	524.36	Joback Method
dvisc	0.0001954	Pa×s	570.97	Joback Method
dvisc	0.0001458	Pa×s	617.59	Joback Method
dvisc	0.0001133	Pa×s	664.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360524&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

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