3-Chlorobenzoic acid, 2-methoxyethyl ester

Inchi: InChI=1S/C10H11ClO3/c1-13-5-6-14-10(12)8-3-2-4-9(11)7-8/h2-4,7H,5-6H2,1H3
InchiKey: WRKWFXODVVARLS-UHFFFAOYSA-N
Formula: C10H11ClO3
SMILES: COCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 214.65

Physical Properties

Property code	Value	Unit	Source
gf	-214.75	kJ/mol	Joback Method
hf	-417.43	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	56.74	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.143		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1580.00		NIST Webbook
rinpol	1580.00		NIST Webbook
tb	596.00	K	Joback Method
tc	811.57	K	Joback Method
tf	365.71	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.40	J/mol×K	596.00	Joback Method
cpg	361.70	J/mol×K	631.93	Joback Method
cpg	373.30	J/mol×K	667.86	Joback Method
cpg	384.22	J/mol×K	703.78	Joback Method
cpg	394.45	J/mol×K	739.71	Joback Method
cpg	403.99	J/mol×K	775.64	Joback Method
cpg	412.84	J/mol×K	811.57	Joback Method
dvisc	0.0012484	Pa×s	365.71	Joback Method

dvisc	0.0007630	Pa×s	404.09	Joback Method
dvisc	0.0005079	Pa×s	442.47	Joback Method
dvisc	0.0003608	Pa×s	480.86	Joback Method
dvisc	0.0002696	Pa×s	519.24	Joback Method
dvisc	0.0002097	Pa×s	557.62	Joback Method
dvisc	0.0001684	Pa×s	596.00	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=U357392&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