

2-Chlorobenzoic acid, 2-methoxyethyl ester

Inchi:	InChI=1S/C10H11ClO3/c1-13-6-7-14-10(12)8-4-2-3-5-9(8)11/h2-5H,6-7H2,1H3
InchiKey:	LIELFQXNPGTYLH-UHFFFAOYSA-N
Formula:	C10H11ClO3
SMILES:	COCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	214.65

Physical Properties

Property code	Value	Unit	Source
hf	-457.46	kJ/mol	Cheméo Relay (1.0)
hfus	23.48	kJ/mol	Joback Method
hvap	73.39	kJ/mol	Cheméo Relay (1.0)
ie	9.04	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	2.143		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1577.00		NIST Webbook
tb	556.39	K	Cheméo Relay (1.0)
tc	761.31	K	Cheméo Relay (1.0)
tf	268.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.40	J/mol×K	596.00	Joback Method
cpg	412.84	J/mol×K	811.57	Joback Method
cpg	403.99	J/mol×K	775.64	Joback Method
cpg	394.45	J/mol×K	739.71	Joback Method
cpg	384.22	J/mol×K	703.78	Joback Method
cpg	373.30	J/mol×K	667.86	Joback Method
cpg	361.70	J/mol×K	631.93	Joback Method
dvisc	0.0003608	Pa×s	480.86	Joback Method
dvisc	0.0001684	Pa×s	596.00	Joback Method
dvisc	0.0002097	Pa×s	557.62	Joback Method

dvisc	0.0002696	Pa×s	519.24	Joback Method
dvisc	0.0012484	Pa×s	365.71	Joback Method
dvisc	0.0005079	Pa×s	442.47	Joback Method
dvisc	0.0007630	Pa×s	404.09	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C501357104&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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