2-((2-Chloroethoxy)carbonyl)benzoic acid

Inchi: InChI=1S/C10H9ClO4/c11-5-6-15-10(14)8-4-2-1-3-7(8)9(12)13/h1-4H,5-6H2,(H,12,13)
InchiKey: YTFGPKHKZPYPFL-UHFFFAOYSA-N
Formula: C10H9ClO4
SMILES: O=C(O)c1ccccc1C(=O)OCCCl
Mol. weight [g/mol]: 228.63
CAS: 6139-60-2

Physical Properties

Property code	Value	Unit	Source
gf	-375.49	kJ/mol	Joback Method
hf	-550.02	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hvap	77.76	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.780		Crippen Method
mcvol	155.120	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	719.63	K	Joback Method
tc	929.26	K	Joback Method
tf	454.23	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.91	J/mol×K	719.63	Joback Method
cpg	391.84	J/mol×K	754.57	Joback Method
cpg	400.11	J/mol×K	789.51	Joback Method
cpg	407.76	J/mol×K	824.45	Joback Method
cpg	414.80	J/mol×K	859.38	Joback Method
cpg	421.23	J/mol×K	894.32	Joback Method
cpg	427.07	J/mol×K	929.26	Joback Method

dvisc	0.0010322	Pa×s	454.23	Joback Method
dvisc	0.0004971	Pa×s	498.46	Joback Method
dvisc	0.0002697	Pa×s	542.70	Joback Method
dvisc	0.0001605	Pa×s	586.93	Joback Method
dvisc	0.0001027	Pa×s	631.16	Joback Method
dvisc	0.0000697	Pa×s	675.40	Joback Method
dvisc	0.0000496	Pa×s	719.63	Joback Method

Sources

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=C6139602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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