2-[(2-Chloropropanoyl)oxy]benzoic acid

Inchi: InChI=1S/C10H9ClO4/c1-6(11)10(14)15-8-5-3-2-4-7(8)9(12)13/h2-6H,1H3,(H,12,13)
InchiKey: RPYJPJMBMJMCRR-UHFFFAOYSA-N
Formula: C10H9ClO4
SMILES: CC(Cl)C(=O)Oc1ccccc1C(=O)O
Mol. weight [g/mol]: 228.63
CAS: 55162-40-8

Physical Properties

Property code	Value	Unit	Source
gf	-377.93	kJ/mol	Joback Method
hf	-555.30	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	77.37	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.917		Crippen Method
mcvol	155.120	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	719.19	K	Joback Method
tc	932.38	K	Joback Method
tf	439.23	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.53	J/mol×K	719.19	Joback Method
cpg	422.36	J/mol×K	896.84	Joback Method
cpg	415.89	J/mol×K	861.31	Joback Method
cpg	408.79	J/mol×K	825.78	Joback Method
cpg	401.04	J/mol×K	790.25	Joback Method
cpg	392.62	J/mol×K	754.72	Joback Method
cpg	428.21	J/mol×K	932.38	Joback Method
dvisc	0.0000458	Pa×s	719.19	Joback Method
dvisc	0.0000660	Pa×s	672.53	Joback Method

dvisc	0.0001003	Pa×s	625.87	Joback Method
dvisc	0.0001631	Pa×s	579.21	Joback Method
dvisc	0.0002888	Pa×s	532.55	Joback Method
dvisc	0.0005707	Pa×s	485.89	Joback Method
dvisc	0.0013033	Pa×s	439.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55162408&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume