Chloroacetic acid, 3-ethylphenyl ester

Inchi: InChI=1S/C10H11ClO2/c1-2-8-4-3-5-9(6-8)13-10(12)7-11/h3-6H,2,7H2,1H3
InchiKey: YRHSYUNQLUKWJD-UHFFFAOYSA-N
Formula: C10H11ClO2
SMILES: CCc1cccc(OC(=O)CCl)c1
Mol. weight [g/mol]: 198.65

Physical Properties

Property code	Value	Unit	Source
gf	-109.75	kJ/mol	Joback Method
hf	-285.21	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	54.33	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.393		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
tb	573.58	K	Joback Method
tc	791.74	K	Joback Method
tf	343.48	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.95	J/mol×K	573.58	Joback Method
cpg	338.44	J/mol×K	609.94	Joback Method
cpg	350.20	J/mol×K	646.30	Joback Method
cpg	361.23	J/mol×K	682.66	Joback Method
cpg	371.57	J/mol×K	719.02	Joback Method
cpg	381.22	J/mol×K	755.38	Joback Method
cpg	390.20	J/mol×K	791.74	Joback Method
dvisc	0.0016661	Pa×s	343.48	Joback Method

dvisc	0.0009919	Pa×s	381.83	Joback Method
dvisc	0.0006491	Pa×s	420.18	Joback Method
dvisc	0.0004560	Pa×s	458.53	Joback Method
dvisc	0.0003383	Pa×s	496.88	Joback Method
dvisc	0.0002619	Pa×s	535.23	Joback Method
dvisc	0.0002099	Pa×s	573.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354610&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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