Octanoic acid, 8-chloro-8-oxo-, ethyl ester

Other names:	Ethyl 8-chloro-8-oxooctanoate
	ethyl 7-chloro-7-formylheptanoate
Inchi:	InChI=1S/C10H17ClO3/c1-2-14-10(13)8-6-4-3-5-7-9(11)12/h2-8H2,1H3
InchiKey:	ZKXJSBHGOFAICL-UHFFFAOYSA-N
Formula:	C10H17ClO3
SMILES:	CCOC(=O)CCCCCCC(=O)Cl
Mol. weight [g/mol]:	220.69
CAS:	14113-02-1

Physical Properties

Property code	Value	Unit	Source
gf	-341.45	kJ/mol	Joback Method
hf	-622.85	kJ/mol	Joback Method
hfus	30.24	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.655		Crippen Method
mcvol	173.010	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1513.00		NIST Webbook
tb	595.79	K	Joback Method
tc	781.25	K	Joback Method
tf	354.47	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.29	J/mol×K	595.79	Joback Method
cpg	431.00	J/mol×K	626.70	Joback Method
cpg	443.12	J/mol×K	657.61	Joback Method
cpg	454.65	J/mol×K	688.52	Joback Method
cpg	465.61	J/mol×K	719.43	Joback Method
cpg	476.00	J/mol×K	750.34	Joback Method

cpg	485.83	J/mol×K	781.25	Joback Method
dvisc	0.0023152	Pa×s	354.47	Joback Method
dvisc	0.0012887	Pa×s	394.69	Joback Method
dvisc	0.0007995	Pa×s	434.91	Joback Method
dvisc	0.0005377	Pa×s	475.13	Joback Method
dvisc	0.0003847	Pa×s	515.35	Joback Method
dvisc	0.0002890	Pa×s	555.57	Joback Method
dvisc	0.0002256	Pa×s	595.79	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=C14113021&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

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