4-chlorooctyl chloroacetate

Other names: 1-Octanol, 4-chloro, chloroacetate
Inchi: InChI=1S/C10H18Cl2O2/c1-2-3-5-9(12)6-4-7-14-10(13)8-11/h9H,2-8H2,1H3
InchiKey: KYSGKJNVTZDICM-UHFFFAOYSA-N
Formula: C10H18Cl2O2
SMILES: CCCCC(Cl)CCCOC(=O)CCl
Mol. weight [g/mol]: 241.16

Physical Properties

Property code	Value	Unit	Source
gf	-226.90	kJ/mol	Joback Method
hf	-531.29	kJ/mol	Joback Method
hfus	29.31	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.346		Crippen Method
mcvol	183.680	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1569.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1575.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2258.00		NIST Webbook
tb	578.91	K	Joback Method
tc	764.42	K	Joback Method
tf	319.46	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.73	J/mol×K	578.91	Joback Method
cpg	441.05	J/mol×K	609.83	Joback Method

cpg	453.75	J/mol×K	640.75	Joback Method
cpg	465.85	J/mol×K	671.67	Joback Method
cpg	477.36	J/mol×K	702.58	Joback Method
cpg	488.28	J/mol×K	733.50	Joback Method
cpg	498.63	J/mol×K	764.42	Joback Method
dvisc	0.0032066	Pa×s	319.46	Joback Method
dvisc	0.0015197	Pa×s	362.70	Joback Method
dvisc	0.0008444	Pa×s	405.94	Joback Method
dvisc	0.0005254	Pa×s	449.19	Joback Method
dvisc	0.0003553	Pa×s	492.43	Joback Method
dvisc	0.0002560	Pa×s	535.67	Joback Method
dvisc	0.0001937	Pa×s	578.91	Joback Method

Sources

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=R112179&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume