Chloroacetic acid, 8-chlorooctyl ester

Other names: 8-chlorooctyl chloroacetate
1-Octanol, 8-chloro, chloroacetate
Inchi: InChI=1S/C10H18Cl2O2/c11-7-5-3-1-2-4-6-8-14-10(13)9-12/h1-9H2
InchiKey: FBWYWOXCNBCYJZ-UHFFFAOYSA-N
Formula: C10H18Cl2O2
SMILES: O=C(CCl)OCCCCCCCCCl
Mol. weight [g/mol]: 241.16

Physical Properties

Property code	Value	Unit	Source
gf	-224.46	kJ/mol	Joback Method
hf	-526.01	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.348		Crippen Method
mcvol	183.680	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1663.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
ripol	2408.00		NIST Webbook
ripol	2425.00		NIST Webbook
ripol	2438.00		NIST Webbook
tb	579.35	K	Joback Method
tc	761.47	K	Joback Method
tf	334.46	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	427.35	J/mol×K	579.35	Joback Method
cpg	440.37	J/mol×K	609.70	Joback Method
cpg	452.81	J/mol×K	640.06	Joback Method
cpg	464.67	J/mol×K	670.41	Joback Method
cpg	475.97	J/mol×K	700.77	Joback Method
cpg	486.72	J/mol×K	731.12	Joback Method
cpg	496.91	J/mol×K	761.47	Joback Method
dvisc	0.0024726	Pa×s	334.46	Joback Method
dvisc	0.0013060	Pa×s	375.28	Joback Method
dvisc	0.0007818	Pa×s	416.09	Joback Method
dvisc	0.0005129	Pa×s	456.90	Joback Method
dvisc	0.0003606	Pa×s	497.72	Joback Method
dvisc	0.0002675	Pa×s	538.53	Joback Method
dvisc	0.0002069	Pa×s	579.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354612&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
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