3-Methylbut-2-enoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C13H23ClO2/c1-12(2)11-13(15)16-10-8-6-4-3-5-7-9-14/h11H,3-10H2,1-2H3
InchiKey: TWGZIXOWCXUULI-UHFFFAOYSA-N
Formula: C13H23ClO2
SMILES: CC(C)=CC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 246.77

Physical Properties

Property code	Value	Unit	Source
gf	-115.60	kJ/mol	Joback Method
hf	-464.76	kJ/mol	Joback Method
hfus	35.30	kJ/mol	Joback Method
hvap	58.11	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.075		Crippen Method
mcvol	209.410	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	1844.00		NIST Webbook
tb	614.60	K	Joback Method
tc	796.78	K	Joback Method
tf	319.31	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.32	J/mol×K	614.60	Joback Method
cpg	542.71	J/mol×K	644.96	Joback Method
cpg	557.38	J/mol×K	675.33	Joback Method
cpg	571.34	J/mol×K	705.69	Joback Method
cpg	584.62	J/mol×K	736.06	Joback Method
cpg	597.25	J/mol×K	766.42	Joback Method
cpg	609.24	J/mol×K	796.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355131&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
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