Isovaleric acid, 8-chlorooctyl ester

Inchi: InChI=1S/C13H25ClO2/c1-12(2)11-13(15)16-10-8-6-4-3-5-7-9-14/h12H,3-11H2,1-2H3
InchiKey: XJVIXTJLJWCUQN-UHFFFAOYSA-N
Formula: C13H25ClO2
SMILES: CC(C)CC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 248.79

Physical Properties

Property code	Value	Unit	Source
gf	-189.71	kJ/mol	Joback Method
hf	-577.47	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	4.155		Crippen Method
mcvol	213.710	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1736.00		NIST Webbook
rinpol	1736.00		NIST Webbook
tb	610.12	K	Joback Method
tc	786.44	K	Joback Method
tf	323.35	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.21	J/mol×K	610.12	Joback Method
cpg	620.96	J/mol×K	757.05	Joback Method
cpg	607.77	J/mol×K	727.67	Joback Method
cpg	593.91	J/mol×K	698.28	Joback Method
cpg	579.37	J/mol×K	668.89	Joback Method
cpg	564.14	J/mol×K	639.51	Joback Method
cpg	633.51	J/mol×K	786.44	Joback Method
dvisc	0.0001484	Pa×s	610.12	Joback Method

dvisc	0.0001991	Pa×s	562.33	Joback Method
dvisc	0.0002822	Pa×s	514.53	Joback Method
dvisc	0.0004297	Pa×s	466.74	Joback Method
dvisc	0.0007200	Pa×s	418.94	Joback Method
dvisc	0.0013781	Pa×s	371.14	Joback Method
dvisc	0.0031957	Pa×s	323.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360657&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