5-chlorovaleric acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C10H17ClO2/c1-9(2)6-8-13-10(12)5-3-4-7-11/h6H,3-5,7-8H2,1-2H3
InchiKey: VWQQVHCGEXKURD-UHFFFAOYSA-N
Formula: C10H17ClO2
SMILES: CC(C)=CCOC(=O)CCCCCl
Mol. weight [g/mol]: 204.70

Physical Properties

Property code	Value	Unit	Source
hf	-511.22	kJ/mol	Cheméo Relay (1.0)
hfus	27.53	kJ/mol	Joback Method
hvap	66.83	kJ/mol	Cheméo Relay (1.0)
ie	9.07	eV	Cheméo Relay (1.0)
log10ws	-3.13		Cheméo Relay (1.0)
logp	2.905		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
rinpol	1459.90		NIST Webbook
rinpol	1459.90		NIST Webbook
tb	513.12	K	Cheméo Relay (1.0)
tc	700.19	K	Cheméo Relay (1.0)
tf	233.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.70	J/mol×K	545.96	Joback Method
cpg	393.10	J/mol×K	577.28	Joback Method
cpg	405.87	J/mol×K	608.59	Joback Method
cpg	418.03	J/mol×K	639.91	Joback Method
cpg	429.60	J/mol×K	671.22	Joback Method
cpg	440.60	J/mol×K	702.54	Joback Method
cpg	451.04	J/mol×K	733.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292474&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point