5-Chlorovaleric acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C17H27ClO2/c18-5-2-1-3-16(19)20-6-4-17-10-13-7-14(11-17)9-15(8-13)12-17/

InchiKey: VZIRUWPGJKHWAM-UHFFFAOYSA-N

Formula: C17H27ClO2

SMILES: O=C(CCCCCl)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 298.85

Physical Properties

Property code	Value	Unit	Source
gf	3.36	kJ/mol	Joback Method
hf	-447.61	kJ/mol	Joback Method
hfus	33.85	kJ/mol	Joback Method
hvap	65.43	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.545		Crippen Method
mcvol	237.490	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2291.40		NIST Webbook
tb	722.14	K	Joback Method
tc	931.08	K	Joback Method
tf	453.39	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.80	J/mol×K	722.14	Joback Method
cpg	744.44	J/mol×K	756.96	Joback Method
cpg	763.22	J/mol×K	791.79	Joback Method
cpg	781.31	J/mol×K	826.61	Joback Method
cpg	798.89	J/mol×K	861.43	Joback Method
cpg	816.13	J/mol×K	896.25	Joback Method
cpg	833.20	J/mol×K	931.08	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=U292245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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