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
hf	-667.13	kJ/mol	Cheméo Relay (1.0)
hfus	33.85	kJ/mol	Joback Method
hvap	92.03	kJ/mol	Cheméo Relay (1.0)
logp	4.545		Crippen Method
mcvol	237.490	ml/mol	McGowan Method
rinpol	2291.40		NIST Webbook

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292245&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):	

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices