5-Chlorovaleric acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C16H25ClO2/c17-4-2-1-3-15(18)19-11-16-8-12-5-13(9-16)7-14(6-12)10-16/h12
InchiKey: VEQDGEGLHTXBCJ-UHFFFAOYSA-N
Formula: C16H25ClO2
SMILES: O=C(CCCCCl)OCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 284.82

Physical Properties

Property code	Value	Unit	Source
gf	-5.06	kJ/mol	Joback Method
hf	-426.97	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	63.20	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.155		Crippen Method
mcvol	223.400	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2154.20		NIST Webbook
rinpol	2154.20		NIST Webbook
tb	699.26	K	Joback Method
tc	911.01	K	Joback Method
tf	442.12	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.37	J/mol×K	699.26	Joback Method
cpg	687.67	J/mol×K	734.55	Joback Method
cpg	706.06	J/mol×K	769.84	Joback Method
cpg	723.70	J/mol×K	805.13	Joback Method
cpg	740.77	J/mol×K	840.43	Joback Method
cpg	757.44	J/mol×K	875.72	Joback Method
cpg	773.89	J/mol×K	911.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292244&Units=SI

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

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