5-Chlorovaleric acid, 2-adamantyl ester

Inchi: InChI=1S/C15H23ClO2/c16-4-2-1-3-14(17)18-15-12-6-10-5-11(8-12)9-13(15)7-10/h10-13
InchiKey: XEDXKFLTKHZQND-UHFFFAOYSA-N
Formula: C15H23ClO2
SMILES: O=C(CCCCCl)OC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 270.80

Physical Properties

Property code	Value	Unit	Source
gf	-15.70	kJ/mol	Joback Method
hf	-441.91	kJ/mol	Joback Method
hfus	36.04	kJ/mol	Joback Method
hvap	61.82	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.763		Crippen Method
mcvol	209.310	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2055.20		NIST Webbook
rinpol	2055.20		NIST Webbook
tb	671.47	K	Joback Method
tc	879.31	K	Joback Method
tf	402.71	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.94	J/mol×K	671.47	Joback Method
cpg	705.02	J/mol×K	844.67	Joback Method
cpg	689.88	J/mol×K	810.03	Joback Method
cpg	673.78	J/mol×K	775.39	Joback Method
cpg	656.65	J/mol×K	740.75	Joback Method
cpg	638.39	J/mol×K	706.11	Joback Method
cpg	719.29	J/mol×K	879.31	Joback Method
dvisc	0.0023890	Pa×s	671.47	Joback Method

dvisc	0.0025016	Pa×s	626.68	Joback Method
dvisc	0.0026383	Pa×s	581.88	Joback Method
dvisc	0.0028071	Pa×s	537.09	Joback Method
dvisc	0.0030207	Pa×s	492.30	Joback Method
dvisc	0.0032987	Pa×s	447.50	Joback Method
dvisc	0.0036734	Pa×s	402.71	Joback Method

Sources

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=U292243&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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