5-Chlorovaleric acid, octadecyl ester

Inchi: InChI=1S/C23H45ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-26-23(25)20-17-
InchiKey: NIFZBQWHRAITQZ-UHFFFAOYSA-N
Formula: C23H45ClO2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCl
Mol. weight [g/mol]: 389.06

Physical Properties

Property code	Value	Unit	Source
gf	-103.07	kJ/mol	Joback Method
hf	-778.59	kJ/mol	Joback Method
hfus	62.31	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	8.200		Crippen Method
mcvol	354.610	ml/mol	McGowan Method
pc	856.47	kPa	Joback Method
tb	839.36	K	Joback Method
tc	1027.66	K	Joback Method
tf	451.05	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.17	J/mol×K	839.36	Joback Method
cpg	1149.50	J/mol×K	870.74	Joback Method
cpg	1168.70	J/mol×K	902.13	Joback Method
cpg	1186.80	J/mol×K	933.51	Joback Method
cpg	1203.85	J/mol×K	964.89	Joback Method
cpg	1219.88	J/mol×K	996.28	Joback Method
cpg	1234.92	J/mol×K	1027.66	Joback Method
dvisc	0.0009116	Pa×s	451.05	Joback Method
dvisc	0.0003940	Pa×s	515.77	Joback Method
dvisc	0.0002053	Pa×s	580.49	Joback Method

dvisc	0.0001219	Pa×s	645.20	Joback Method
dvisc	0.0000796	Pa×s	709.92	Joback Method
dvisc	0.0000558	Pa×s	774.64	Joback Method
dvisc	0.0000414	Pa×s	839.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292318&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume