5-Chlorovaleric acid, hexadecyl ester

Inchi: InChI=1S/C21H41ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-24-21(23)18-15-16-19-
InchiKey: HJPJQMNZOQVLCN-UHFFFAOYSA-N
Formula: C21H41ClO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCl
Mol. weight [g/mol]: 361.00

Physical Properties

Property code	Value	Unit	Source
gf	-119.91	kJ/mol	Joback Method
hf	-737.31	kJ/mol	Joback Method
hfus	57.13	kJ/mol	Joback Method
hvap	75.88	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	7.420		Crippen Method
mcvol	326.430	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	2565.10		NIST Webbook
tb	793.60	K	Joback Method
tc	973.90	K	Joback Method
tf	428.51	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.07	J/mol×K	793.60	Joback Method
cpg	1024.39	J/mol×K	823.65	Joback Method
cpg	1042.70	J/mol×K	853.70	Joback Method
cpg	1060.04	J/mol×K	883.75	Joback Method
cpg	1076.44	J/mol×K	913.80	Joback Method
cpg	1091.93	J/mol×K	943.85	Joback Method
cpg	1106.54	J/mol×K	973.90	Joback Method
dvisc	0.0011536	Pa×s	428.51	Joback Method
dvisc	0.0005079	Pa×s	489.36	Joback Method

dvisc	0.0002681	Pa×s	550.21	Joback Method
dvisc	0.0001607	Pa×s	611.05	Joback Method
dvisc	0.0001057	Pa×s	671.90	Joback Method
dvisc	0.0000745	Pa×s	732.75	Joback Method
dvisc	0.0000554	Pa×s	793.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292317&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume