5-Chlorovaleric acid, heptadecyl ester

Inchi: InChI=1S/C22H43ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-25-22(24)19-16-17-
InchiKey: DBESYZFSKKRNPR-UHFFFAOYSA-N
Formula: C22H43ClO2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCCCl
Mol. weight [g/mol]: 375.03

Physical Properties

Property code	Value	Unit	Source
gf	-111.49	kJ/mol	Joback Method
hf	-757.95	kJ/mol	Joback Method
hfus	59.72	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.810		Crippen Method
mcvol	340.520	ml/mol	McGowan Method
pc	906.70	kPa	Joback Method
rinpol	2621.10		NIST Webbook
tb	816.48	K	Joback Method
tc	1000.37	K	Joback Method
tf	439.78	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.74	J/mol×K	816.48	Joback Method
cpg	1086.54	J/mol×K	847.13	Joback Method
cpg	1105.29	J/mol×K	877.78	Joback Method
cpg	1123.00	J/mol×K	908.43	Joback Method
cpg	1139.72	J/mol×K	939.07	Joback Method
cpg	1155.47	J/mol×K	969.72	Joback Method
cpg	1170.29	J/mol×K	1000.37	Joback Method
dvisc	0.0010274	Pa×s	439.78	Joback Method
dvisc	0.0004480	Pa×s	502.56	Joback Method

dvisc	0.0002349	Pa×s	565.35	Joback Method
dvisc	0.0001402	Pa×s	628.13	Joback Method
dvisc	0.0000918	Pa×s	690.91	Joback Method
dvisc	0.0000646	Pa×s	753.70	Joback Method
dvisc	0.0000479	Pa×s	816.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292249&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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