2-chloroethyl eicosanoate

Inchi: InChI=1S/C22H43ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22(24)25-21-
InchiKey: XAARWHAYKZHMOM-UHFFFAOYSA-N
Formula: C22H43ClO2
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)OCCCl
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	2611.00		NIST Webbook
rinpol	2614.00		NIST Webbook
rinpol	2611.00		NIST Webbook
ripol	3100.00		NIST Webbook
ripol	3111.00		NIST Webbook
ripol	3108.00		NIST Webbook
ripol	3100.00		NIST Webbook
ripol	3102.00		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	1155.47	J/mol×K	969.72	Joback Method

cpg	1139.72	J/mol×K	939.07	Joback Method
cpg	1123.00	J/mol×K	908.43	Joback Method
cpg	1105.29	J/mol×K	877.78	Joback Method
cpg	1086.54	J/mol×K	847.13	Joback Method
cpg	1170.29	J/mol×K	1000.37	Joback Method
dvisc	0.0000479	Pa×s	816.48	Joback Method
dvisc	0.0000646	Pa×s	753.70	Joback Method
dvisc	0.0000918	Pa×s	690.91	Joback Method
dvisc	0.0001402	Pa×s	628.13	Joback Method
dvisc	0.0002349	Pa×s	565.35	Joback Method
dvisc	0.0004480	Pa×s	502.56	Joback Method
dvisc	0.0010274	Pa×s	439.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30773&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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