1,2-Cyclohexanedicarboxylic acid, 2-chloroethyl undecyl ester

Inchi: InChI=1S/C21H37ClO4/c1-2-3-4-5-6-7-8-9-12-16-25-20(23)18-13-10-11-14-19(18)21(24)26-17-15-22/h18-19H,2-17H2,1H3

InchiKey: DXMZDAHEIVWOBD-UHFFFAOYSA-N

Formula: C21H37ClO4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCl

Mol. weight [g/mol]: 388.97

Physical Properties

Property code	Value	Unit	Source
gf	-337.09	kJ/mol	Joback Method
hf	-948.13	kJ/mol	Joback Method
hfus	52.82	kJ/mol	Joback Method
hvap	85.16	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.649		Crippen Method
mcvol	323.010	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinpol	2675.00		NIST Webbook
rinpol	2675.00		NIST Webbook
tb	884.77	K	Joback Method
tc	1087.55	K	Joback Method
tf	503.81	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.09	J/mol×K	884.77	Joback Method
cpg	1080.14	J/mol×K	918.57	Joback Method
cpg	1096.75	J/mol×K	952.36	Joback Method
cpg	1111.95	J/mol×K	986.16	Joback Method
cpg	1125.78	J/mol×K	1019.96	Joback Method
cpg	1138.24	J/mol×K	1053.75	Joback Method
cpg	1149.37	J/mol×K	1087.55	Joback Method
dvisc	0.0007293	Pa×s	503.81	Joback Method

dvisc	0.0003686	Pa×s	567.30	Joback Method
dvisc	0.0002137	Pa×s	630.80	Joback Method
dvisc	0.0001369	Pa×s	694.29	Joback Method
dvisc	0.0000945	Pa×s	757.78	Joback Method
dvisc	0.0000691	Pa×s	821.28	Joback Method
dvisc	0.0000528	Pa×s	884.77	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=U340050&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

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