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

Inchi: InChI=1S/C22H39ClO4/c1-2-3-4-5-6-7-8-9-10-13-17-26-21(24)19-14-11-12-15-20(19)22(
InchiKey: QDGLGTBGQBDRQZ-UHFFFAOYSA-N
Formula: C22H39ClO4
SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCl
Mol. weight [g/mol]: 403.00

Physical Properties

Property code	Value	Unit	Source
gf	-328.67	kJ/mol	Joback Method
hf	-968.77	kJ/mol	Joback Method
hfus	55.41	kJ/mol	Joback Method
hvap	87.38	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	6.039		Crippen Method
mcvol	337.100	ml/mol	McGowan Method
pc	1038.57	kPa	Joback Method
rinpol	2777.00		NIST Webbook
rinpol	2777.00		NIST Webbook
tb	907.65	K	Joback Method
tc	1113.21	K	Joback Method
tf	515.08	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.87	J/mol×K	907.65	Joback Method
cpg	1199.88	J/mol×K	1078.95	Joback Method
cpg	1187.57	J/mol×K	1044.69	Joback Method
cpg	1173.84	J/mol×K	1010.43	Joback Method
cpg	1158.66	J/mol×K	976.17	Joback Method
cpg	1142.01	J/mol×K	941.91	Joback Method
cpg	1210.79	J/mol×K	1113.21	Joback Method
dvisc	0.0000456	Pa×s	907.65	Joback Method

dvisc	0.0000597	Pa×s	842.22	Joback Method
dvisc	0.0000820	Pa×s	776.79	Joback Method
dvisc	0.0001193	Pa×s	711.37	Joback Method
dvisc	0.0001873	Pa×s	645.94	Joback Method
dvisc	0.0003254	Pa×s	580.51	Joback Method
dvisc	0.0006506	Pa×s	515.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340051&Units=SI

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