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

Inchi: InChI=1S/C25H45ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-20-29-24(27)22-17-14-15-18-

InchiKey: IVIGWIZYOYEFDM-UHFFFAOYSA-N

Formula: C25H45ClO4

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

Mol. weight [g/mol]: 445.07

Physical Properties

Property code	Value	Unit	Source
gf	-303.41	kJ/mol	Joback Method
hf	-1030.69	kJ/mol	Joback Method
hfus	63.18	kJ/mol	Joback Method
hvap	94.06	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	7.209		Crippen Method
mcvol	379.370	ml/mol	McGowan Method
pc	869.65	kPa	Joback Method
rinpol	3118.00		NIST Webbook
rinpol	3118.00		NIST Webbook
tb	976.29	K	Joback Method
tc	1195.75	K	Joback Method
tf	548.89	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1311.90	J/mol×K	976.29	Joback Method
cpg	1330.47	J/mol×K	1012.87	Joback Method
cpg	1347.25	J/mol×K	1049.44	Joback Method
cpg	1362.28	J/mol×K	1086.02	Joback Method
cpg	1375.60	J/mol×K	1122.60	Joback Method
cpg	1387.26	J/mol×K	1159.18	Joback Method
cpg	1397.30	J/mol×K	1195.75	Joback Method
dvisc	0.0004531	Pa×s	548.89	Joback Method

dvisc	0.0002202	Pa×s	620.12	Joback Method
dvisc	0.0001241	Pa×s	691.36	Joback Method
dvisc	0.0000779	Pa×s	762.59	Joback Method
dvisc	0.0000529	Pa×s	833.82	Joback Method
dvisc	0.0000382	Pa×s	905.06	Joback Method
dvisc	0.0000289	Pa×s	976.29	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=U340053&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