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

Inchi: InChI=1S/C24H43ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-15-19-28-23(26)21-16-13-14-17-22(

InchiKey: IORCAXGUDIKWPG-UHFFFAOYSA-N

Formula: C24H43ClO4

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

Mol. weight [g/mol]: 431.05

Physical Properties

Property code	Value	Unit	Source
gf	-311.83	kJ/mol	Joback Method
hf	-1010.05	kJ/mol	Joback Method
hfus	60.59	kJ/mol	Joback Method
hvap	91.83	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.819		Crippen Method
mcvol	365.280	ml/mol	McGowan Method
pc	921.06	kPa	Joback Method
rinpol	2996.00		NIST Webbook
rinpol	2996.00		NIST Webbook
tb	953.41	K	Joback Method
tc	1167.24	K	Joback Method
tf	537.62	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.83	J/mol×K	953.41	Joback Method
cpg	1267.24	J/mol×K	989.05	Joback Method
cpg	1283.97	J/mol×K	1024.69	Joback Method
cpg	1299.05	J/mol×K	1060.33	Joback Method
cpg	1312.53	J/mol×K	1095.96	Joback Method
cpg	1324.44	J/mol×K	1131.60	Joback Method
cpg	1334.82	J/mol×K	1167.24	Joback Method
dvisc	0.0005127	Pa×s	537.62	Joback Method

dvisc	0.0002515	Pa×s	606.92	Joback Method
dvisc	0.0001427	Pa×s	676.22	Joback Method
dvisc	0.0000900	Pa×s	745.51	Joback Method
dvisc	0.0000614	Pa×s	814.81	Joback Method
dvisc	0.0000444	Pa×s	884.11	Joback Method
dvisc	0.0000337	Pa×s	953.41	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=U340052&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