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

Inchi: InChI=1S/C16H27ClO4/c1-12(2)6-5-10-20-15(18)13-7-3-4-8-14(13)16(19)21-11-9-17/h12
InchiKey: CUNQUAKHJJETDW-UHFFFAOYSA-N
Formula: C16H27ClO4
SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OCCCl
Mol. weight [g/mol]: 318.84

Physical Properties

Property code	Value	Unit	Source
gf	-381.63	kJ/mol	Joback Method
hf	-850.21	kJ/mol	Joback Method
hfus	36.35	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.554		Crippen Method
mcvol	252.560	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	769.93	K	Joback Method
tc	972.68	K	Joback Method
tf	432.46	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.45	J/mol×K	769.93	Joback Method
cpg	781.20	J/mol×K	803.72	Joback Method
cpg	797.72	J/mol×K	837.51	Joback Method
cpg	813.03	J/mol×K	871.30	Joback Method
cpg	827.13	J/mol×K	905.10	Joback Method
cpg	840.04	J/mol×K	938.89	Joback Method
cpg	851.75	J/mol×K	972.68	Joback Method
dvisc	0.0014210	Pa×s	432.46	Joback Method

dvisc	0.0007040	Pa×s	488.70	Joback Method
dvisc	0.0004032	Pa×s	544.95	Joback Method
dvisc	0.0002563	Pa×s	601.19	Joback Method
dvisc	0.0001760	Pa×s	657.44	Joback Method
dvisc	0.0001283	Pa×s	713.68	Joback Method
dvisc	0.0000979	Pa×s	769.93	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=U340044&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