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

Inchi: InChI=1S/C14H23ClO4/c1-10(2)9-19-14(17)12-6-4-3-5-11(12)13(16)18-8-7-15/h10-12H,3
InchiKey: VZDFGACGGMQVTK-UHFFFAOYSA-N
Formula: C14H23ClO4
SMILES: CC(C)COC(=O)C1CCCCC1C(=O)OCCCl
Mol. weight [g/mol]: 290.78

Physical Properties

Property code	Value	Unit	Source
gf	-398.47	kJ/mol	Joback Method
hf	-808.93	kJ/mol	Joback Method
hfus	31.17	kJ/mol	Joback Method
hvap	69.19	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.774		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1916.00		NIST Webbook
rinpol	1916.00		NIST Webbook
tb	724.17	K	Joback Method
tc	930.67	K	Joback Method
tf	409.92	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.70	J/mol×K	724.17	Joback Method
cpg	667.13	J/mol×K	758.59	Joback Method
cpg	683.40	J/mol×K	793.00	Joback Method
cpg	698.53	J/mol×K	827.42	Joback Method
cpg	712.51	J/mol×K	861.84	Joback Method
cpg	725.35	J/mol×K	896.25	Joback Method
cpg	737.05	J/mol×K	930.67	Joback Method
dvisc	0.0017048	Pa×s	409.92	Joback Method

dvisc	0.0008659	Pa×s	462.30	Joback Method
dvisc	0.0005049	Pa×s	514.67	Joback Method
dvisc	0.0003252	Pa×s	567.04	Joback Method
dvisc	0.0002256	Pa×s	619.42	Joback Method
dvisc	0.0001657	Pa×s	671.79	Joback Method
dvisc	0.0001273	Pa×s	724.17	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=U340041&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