1,2-Cyclohexanedicarboxylic acid, (2-chlorocyclohexyl)methyl octyl ester

Inchi: InChI=1S/C23H39ClO4/c1-2-3-4-5-6-11-16-27-22(25)19-13-8-9-14-20(19)23(26)28-17-18
InchiKey: BPQIESLONFQBEA-UHFFFAOYSA-N
Formula: C23H39ClO4
SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1Cl
Mol. weight [g/mol]: 415.01

Physical Properties

Property code	Value	Unit	Source
gf	-303.51	kJ/mol	Joback Method
hf	-955.43	kJ/mol	Joback Method
hfus	50.91	kJ/mol	Joback Method
hvap	89.73	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	6.037		Crippen Method
mcvol	340.330	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2908.00		NIST Webbook
rinpol	2908.00		NIST Webbook
tb	945.41	K	Joback Method
tc	1164.10	K	Joback Method
tf	529.49	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.24	J/mol×K	945.41	Joback Method
cpg	1204.39	J/mol×K	981.86	Joback Method
cpg	1220.60	J/mol×K	1018.31	Joback Method
cpg	1234.93	J/mol×K	1054.75	Joback Method
cpg	1247.38	J/mol×K	1091.20	Joback Method
cpg	1258.01	J/mol×K	1127.65	Joback Method
cpg	1266.82	J/mol×K	1164.10	Joback Method
dvisc	0.0007276	Pa×s	529.49	Joback Method

dvisc	0.0003664	Pa×s	598.81	Joback Method
dvisc	0.0002128	Pa×s	668.13	Joback Method
dvisc	0.0001369	Pa×s	737.45	Joback Method
dvisc	0.0000950	Pa×s	806.77	Joback Method
dvisc	0.0000698	Pa×s	876.09	Joback Method
dvisc	0.0000537	Pa×s	945.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339864&Units=SI
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

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