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

Inchi: InChI=1S/C20H33ClO4/c1-2-3-8-13-24-19(22)16-10-5-6-11-17(16)20(23)25-14-15-9-4-7-

InchiKey: RYVGHSURQYMIMD-UHFFFAOYSA-N

Formula: C20H33ClO4

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1Cl

Mol. weight [g/mol]: 372.93

Physical Properties

Property code	Value	Unit	Source
gf	-328.77	kJ/mol	Joback Method
hf	-893.51	kJ/mol	Joback Method
hfus	43.14	kJ/mol	Joback Method
hvap	83.05	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.867		Crippen Method
mcvol	298.060	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	876.77	K	Joback Method
tc	1094.35	K	Joback Method
tf	495.68	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.96	J/mol×K	876.77	Joback Method
cpg	1019.87	J/mol×K	913.03	Joback Method
cpg	1036.97	J/mol×K	949.30	Joback Method
cpg	1052.31	J/mol×K	985.56	Joback Method
cpg	1065.89	J/mol×K	1021.82	Joback Method
cpg	1077.74	J/mol×K	1058.08	Joback Method
cpg	1087.87	J/mol×K	1094.35	Joback Method
dvisc	0.0010063	Pa×s	495.68	Joback Method

dvisc	0.0005232	Pa×s	559.20	Joback Method
dvisc	0.0003108	Pa×s	622.71	Joback Method
dvisc	0.0002033	Pa×s	686.23	Joback Method
dvisc	0.0001429	Pa×s	749.74	Joback Method
dvisc	0.0001062	Pa×s	813.25	Joback Method
dvisc	0.0000823	Pa×s	876.77	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=U339861&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