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

Inchi: InChI=1S/C22H34Cl2O4/c23-19-11-5-1-7-15(19)13-27-21(25)17-9-3-4-10-18(17)22(26)2

InchiKey: BRNANSGAGKELCH-UHFFFAOYSA-N

Formula: C22H34Cl2O4

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

Mol. weight [g/mol]: 433.41

Physical Properties

Property code	Value	Unit	Source
gf	-307.12	kJ/mol	Joback Method
hf	-916.55	kJ/mol	Joback Method
hfus	45.42	kJ/mol	Joback Method
hvap	92.01	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.474		Crippen Method
mcvol	327.620	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	3183.00		NIST Webbook
tb	974.84	K	Joback Method
tc	1215.22	K	Joback Method
tf	551.28	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.44	J/mol×K	974.84	Joback Method
cpg	1166.97	J/mol×K	1014.90	Joback Method
cpg	1181.03	J/mol×K	1054.97	Joback Method
cpg	1192.64	J/mol×K	1095.03	Joback Method
cpg	1201.84	J/mol×K	1135.10	Joback Method
cpg	1208.66	J/mol×K	1175.16	Joback Method
cpg	1213.14	J/mol×K	1215.22	Joback Method
dvisc	0.0008321	Pa×s	551.28	Joback Method
dvisc	0.0004403	Pa×s	621.87	Joback Method

dvisc	0.0002653	Pa×s	692.47	Joback Method
dvisc	0.0001755	Pa×s	763.06	Joback Method
dvisc	0.0001246	Pa×s	833.65	Joback Method
dvisc	0.0000933	Pa×s	904.25	Joback Method
dvisc	0.0000728	Pa×s	974.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339865&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