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

Inchi: InChI=1S/C22H37ClO4/c1-2-3-4-5-10-15-26-21(24)18-12-7-8-13-19(18)22(25)27-16-17-1

InchiKey: JDTGCOOJAVKGSY-UHFFFAOYSA-N

Formula: C22H37ClO4

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

Mol. weight [g/mol]: 400.98

Physical Properties

Property code	Value	Unit	Source
gf	-311.93	kJ/mol	Joback Method
hf	-934.79	kJ/mol	Joback Method
hfus	48.32	kJ/mol	Joback Method
hvap	87.50	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.647		Crippen Method
mcvol	326.240	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2808.00		NIST Webbook
rinpol	2808.00		NIST Webbook
tb	922.53	K	Joback Method
tc	1140.05	K	Joback Method
tf	518.22	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.07	J/mol×K	922.53	Joback Method
cpg	1197.58	J/mol×K	1103.80	Joback Method
cpg	1186.52	J/mol×K	1067.54	Joback Method
cpg	1173.66	J/mol×K	1031.29	Joback Method
cpg	1158.99	J/mol×K	995.04	Joback Method
cpg	1142.47	J/mol×K	958.78	Joback Method
cpg	1206.88	J/mol×K	1140.05	Joback Method
dvisc	0.0000621	Pa×s	922.53	Joback Method

dvisc	0.0000805	Pa×s	855.14	Joback Method
dvisc	0.0001091	Pa×s	787.76	Joback Method
dvisc	0.0001566	Pa×s	720.38	Joback Method
dvisc	0.0002421	Pa×s	652.99	Joback Method
dvisc	0.0004140	Pa×s	585.61	Joback Method
dvisc	0.0008136	Pa×s	518.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339863&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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