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

Inchi: InChI=1S/C21H35ClO4/c1-15(2)8-7-13-25-20(23)17-10-4-5-11-18(17)21(24)26-14-16-9-3

InchiKey: BCRIHSBUEDJNGV-UHFFFAOYSA-N

Formula: C21H35ClO4

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

Mol. weight [g/mol]: 386.95

Physical Properties

Property code	Value	Unit	Source
gf	-322.79	kJ/mol	Joback Method
hf	-919.43	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.113		Crippen Method
mcvol	312.150	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2658.00		NIST Webbook
rinpol	2658.00		NIST Webbook
tb	899.21	K	Joback Method
tc	1118.49	K	Joback Method
tf	491.95	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.74	J/mol×K	899.21	Joback Method
cpg	1081.54	J/mol×K	935.76	Joback Method
cpg	1098.47	J/mol×K	972.30	Joback Method
cpg	1113.53	J/mol×K	1008.85	Joback Method
cpg	1126.77	J/mol×K	1045.40	Joback Method
cpg	1138.21	J/mol×K	1081.95	Joback Method
cpg	1147.86	J/mol×K	1118.49	Joback Method
dvisc	0.0010224	Pa×s	491.95	Joback Method

dvisc	0.0004897	Pa×s	559.83	Joback Method
dvisc	0.0002750	Pa×s	627.70	Joback Method
dvisc	0.0001729	Pa×s	695.58	Joback Method
dvisc	0.0001180	Pa×s	763.46	Joback Method
dvisc	0.0000858	Pa×s	831.33	Joback Method
dvisc	0.0000654	Pa×s	899.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339862&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