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

Inchi: InChI=1S/C17H27ClO4/c1-2-21-16(19)13-8-4-5-9-14(13)17(20)22-11-12-7-3-6-10-15(12)

InchiKey: SGYFWXNKKCRNJO-UHFFFAOYSA-N

Formula: C17H27ClO4

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

Mol. weight [g/mol]: 330.85

Physical Properties

Property code	Value	Unit	Source
gf	-354.03	kJ/mol	Joback Method
hf	-831.59	kJ/mol	Joback Method
hfus	35.37	kJ/mol	Joback Method
hvap	76.37	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.697		Crippen Method
mcvol	255.790	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
tb	808.13	K	Joback Method
tc	1031.05	K	Joback Method
tf	461.87	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.35	J/mol×K	808.13	Joback Method
cpg	839.95	J/mol×K	845.28	Joback Method
cpg	857.82	J/mol×K	882.44	Joback Method
cpg	873.98	J/mol×K	919.59	Joback Method
cpg	888.44	J/mol×K	956.74	Joback Method
cpg	901.22	J/mol×K	993.90	Joback Method
cpg	912.31	J/mol×K	1031.05	Joback Method
dvisc	0.0013411	Pa×s	461.87	Joback Method

dvisc	0.0007225	Pa×s	519.58	Joback Method
dvisc	0.0004405	Pa×s	577.29	Joback Method
dvisc	0.0002938	Pa×s	635.00	Joback Method
dvisc	0.0002096	Pa×s	692.71	Joback Method
dvisc	0.0001576	Pa×s	750.42	Joback Method
dvisc	0.0001234	Pa×s	808.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339858&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