1,2-Cyclohexanedicarboxylic acid, 4-chloro-3-methylphenyl ethyl ester

Inchi: InChI=1S/C17H21ClO4/c1-3-21-16(19)13-6-4-5-7-14(13)17(20)22-12-8-9-15(18)11(2)10-

InchiKey: DSGYJPIHUBWYTG-UHFFFAOYSA-N

Formula: C17H21ClO4

SMILES: CCOC(=O)C1CCCCC1C(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-277.62	kJ/mol	Joback Method
hf	-651.98	kJ/mol	Joback Method
hfus	35.73	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.923		Crippen Method
mcvol	242.890	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	829.89	K	Joback Method
tc	1059.65	K	Joback Method
tf	510.19	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.07	J/mol×K	829.89	Joback Method
cpg	792.14	J/mol×K	1021.36	Joback Method
cpg	782.26	J/mol×K	983.07	Joback Method
cpg	770.93	J/mol×K	944.77	Joback Method
cpg	758.13	J/mol×K	906.48	Joback Method
cpg	743.84	J/mol×K	868.18	Joback Method
cpg	800.57	J/mol×K	1059.65	Joback Method
dvisc	0.0000974	Pa×s	829.89	Joback Method

dvisc	0.0001210	Pa×s	776.61	Joback Method
dvisc	0.0001552	Pa×s	723.32	Joback Method
dvisc	0.0002072	Pa×s	670.04	Joback Method
dvisc	0.0002907	Pa×s	616.76	Joback Method
dvisc	0.0004349	Pa×s	563.47	Joback Method
dvisc	0.0007076	Pa×s	510.19	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=U339683&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