cis-Cyclohex-4-en-1,2-dicarboxylic acid, 4-chloro-3-methylphenyl ethyl ester

Inchi: InChI=1S/C17H19ClO4/c1-3-21-16(19)13-6-4-5-7-14(13)17(20)22-12-8-9-15(18)11(2)10-

InchiKey: DWLQZUVJDFCJED-UHFFFAOYSA-N

Formula: C17H19ClO4

SMILES: CCOC(=O)C1CC=CCC1C(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 322.78

Physical Properties

Property code	Value	Unit	Source
gf	-247.66	kJ/mol	Joback Method
hf	-594.20	kJ/mol	Joback Method
hfus	36.95	kJ/mol	Joback Method
hvap	80.14	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.699		Crippen Method
mcvol	238.590	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	829.05	K	Joback Method
tc	1060.39	K	Joback Method
tf	510.95	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.20	J/mol×K	829.05	Joback Method
cpg	760.57	J/mol×K	1021.83	Joback Method
cpg	751.33	J/mol×K	983.27	Joback Method
cpg	740.68	J/mol×K	944.72	Joback Method
cpg	728.62	J/mol×K	906.16	Joback Method
cpg	715.13	J/mol×K	867.61	Joback Method
cpg	768.42	J/mol×K	1060.39	Joback Method
dvisc	0.0001048	Pa×s	829.05	Joback Method

dvisc	0.0001291	Pa×s	776.03	Joback Method
dvisc	0.0001640	Pa×s	723.02	Joback Method
dvisc	0.0002163	Pa×s	670.00	Joback Method
dvisc	0.0002993	Pa×s	616.98	Joback Method
dvisc	0.0004401	Pa×s	563.97	Joback Method
dvisc	0.0007010	Pa×s	510.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382645&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

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