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

Inchi: InChI=1S/C21H27ClO4/c1-14(2)7-6-12-25-20(23)17-8-4-5-9-18(17)21(24)26-16-10-11-19

InchiKey: BQKFMTAKHDLQLJ-UHFFFAOYSA-N

Formula: C21H27ClO4

SMILES: Cc1cc(OC(=O)C2CC=CCC2C(=O)OCCCC(C)C)ccc1Cl

Mol. weight [g/mol]: 378.89

Physical Properties

Property code	Value	Unit	Source
gf	-216.42	kJ/mol	Joback Method
hf	-682.04	kJ/mol	Joback Method
hfus	43.78	kJ/mol	Joback Method
hvap	88.66	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.116		Crippen Method
mcvol	294.950	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
tb	920.13	K	Joback Method
tc	1146.27	K	Joback Method
tf	541.03	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.69	J/mol×K	920.13	Joback Method
cpg	947.60	J/mol×K	957.82	Joback Method
cpg	960.93	J/mol×K	995.51	Joback Method
cpg	972.69	J/mol×K	1033.20	Joback Method
cpg	982.91	J/mol×K	1070.89	Joback Method
cpg	991.61	J/mol×K	1108.58	Joback Method
cpg	998.83	J/mol×K	1146.27	Joback Method
dvisc	0.0005303	Pa×s	541.03	Joback Method

dvisc	0.0003001	Pa×s	604.21	Joback Method
dvisc	0.0001892	Pa×s	667.40	Joback Method
dvisc	0.0001292	Pa×s	730.58	Joback Method
dvisc	0.0000937	Pa×s	793.76	Joback Method
dvisc	0.0000713	Pa×s	856.95	Joback Method
dvisc	0.0000563	Pa×s	920.13	Joback Method

Sources

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=U382650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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