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

Inchi: InChI=1S/C21H27ClO4/c1-3-4-5-8-13-25-20(23)17-9-6-7-10-18(17)21(24)26-16-11-12-19

InchiKey: UFKCGOZAOHSYHY-UHFFFAOYSA-N

Formula: C21H27ClO4

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

Mol. weight [g/mol]: 378.89

Physical Properties

Property code	Value	Unit	Source
gf	-213.98	kJ/mol	Joback Method
hf	-676.76	kJ/mol	Joback Method
hfus	47.31	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.260		Crippen Method
mcvol	294.950	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
tb	920.57	K	Joback Method
tc	1144.42	K	Joback Method
tf	556.03	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.20	J/mol×K	920.57	Joback Method
cpg	947.01	J/mol×K	957.88	Joback Method
cpg	960.28	J/mol×K	995.19	Joback Method
cpg	972.02	J/mol×K	1032.50	Joback Method
cpg	982.26	J/mol×K	1069.81	Joback Method
cpg	991.03	J/mol×K	1107.11	Joback Method
cpg	998.36	J/mol×K	1144.42	Joback Method
dvisc	0.0004891	Pa×s	556.03	Joback Method

dvisc	0.0002922	Pa×s	616.79	Joback Method
dvisc	0.0001915	Pa×s	677.54	Joback Method
dvisc	0.0001345	Pa×s	738.30	Joback Method
dvisc	0.0000997	Pa×s	799.06	Joback Method
dvisc	0.0000771	Pa×s	859.81	Joback Method
dvisc	0.0000617	Pa×s	920.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382651&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