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

Inchi: InChI=1S/C20H25ClO4/c1-3-4-7-12-24-19(22)16-8-5-6-9-17(16)20(23)25-15-10-11-18(21

InchiKey: DLEFENZZYQFVGZ-UHFFFAOYSA-N

Formula: C20H25ClO4

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

Mol. weight [g/mol]: 364.86

Physical Properties

Property code	Value	Unit	Source
gf	-222.40	kJ/mol	Joback Method
hf	-656.12	kJ/mol	Joback Method
hfus	44.72	kJ/mol	Joback Method
hvap	86.82	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.870		Crippen Method
mcvol	280.860	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	897.69	K	Joback Method
tc	1122.35	K	Joback Method
tf	544.76	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.20	J/mol×K	897.69	Joback Method
cpg	932.66	J/mol×K	1084.91	Joback Method
cpg	923.71	J/mol×K	1047.47	Joback Method
cpg	913.32	J/mol×K	1010.02	Joback Method
cpg	901.45	J/mol×K	972.58	Joback Method
cpg	888.08	J/mol×K	935.13	Joback Method
cpg	940.18	J/mol×K	1122.35	Joback Method
dvisc	0.0000707	Pa×s	897.69	Joback Method

dvisc	0.0000881	Pa×s	838.87	Joback Method
dvisc	0.0001135	Pa×s	780.05	Joback Method
dvisc	0.0001523	Pa×s	721.22	Joback Method
dvisc	0.0002153	Pa×s	662.40	Joback Method
dvisc	0.0003257	Pa×s	603.58	Joback Method
dvisc	0.0005387	Pa×s	544.76	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=U382649&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