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

Inchi: InChI=1S/C20H27ClO4/c1-3-4-7-12-24-19(22)16-8-5-6-9-17(16)20(23)25-15-10-11-18(21

InchiKey: WKQMDOFIKIRICE-UHFFFAOYSA-N

Formula: C20H27ClO4

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

Mol. weight [g/mol]: 366.88

Physical Properties

Property code	Value	Unit	Source
gf	-252.36	kJ/mol	Joback Method
hf	-713.90	kJ/mol	Joback Method
hfus	43.50	kJ/mol	Joback Method
hvap	86.53	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.094		Crippen Method
mcvol	285.160	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
tb	898.53	K	Joback Method
tc	1122.11	K	Joback Method
tf	544.00	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.77	J/mol×K	898.53	Joback Method
cpg	918.37	J/mol×K	935.79	Joback Method
cpg	932.40	J/mol×K	973.06	Joback Method
cpg	944.89	J/mol×K	1010.32	Joback Method
cpg	955.84	J/mol×K	1047.58	Joback Method
cpg	965.29	J/mol×K	1084.84	Joback Method
cpg	973.25	J/mol×K	1122.11	Joback Method
dvisc	0.0005370	Pa×s	544.00	Joback Method

dvisc	0.0003180	Pa×s	603.09	Joback Method
dvisc	0.0002068	Pa×s	662.18	Joback Method
dvisc	0.0001443	Pa×s	721.26	Joback Method
dvisc	0.0001063	Pa×s	780.35	Joback Method
dvisc	0.0000818	Pa×s	839.44	Joback Method
dvisc	0.0000651	Pa×s	898.53	Joback Method

Sources

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=U339687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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