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

Inchi: InChI=1S/C25H35ClO4/c1-3-4-5-6-7-8-9-12-17-29-24(27)21-13-10-11-14-22(21)25(28)30

InchiKey: IOHLKWVNAHDGLC-UHFFFAOYSA-N

Formula: C25H35ClO4

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

Mol. weight [g/mol]: 435.00

Physical Properties

Property code	Value	Unit	Source
gf	-180.30	kJ/mol	Joback Method
hf	-759.32	kJ/mol	Joback Method
hfus	57.67	kJ/mol	Joback Method
hvap	97.95	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	6.820		Crippen Method
mcvol	351.310	ml/mol	McGowan Method
pc	1072.17	kPa	Joback Method
rinpol	3115.00		NIST Webbook
rinpol	3115.00		NIST Webbook
tb	1012.09	K	Joback Method
tc	1241.03	K	Joback Method
tf	601.11	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1173.19	J/mol×K	1012.09	Joback Method
cpg	1228.44	J/mol×K	1202.87	Joback Method
cpg	1220.72	J/mol×K	1164.72	Joback Method
cpg	1211.38	J/mol×K	1126.56	Joback Method
cpg	1200.37	J/mol×K	1088.40	Joback Method
cpg	1187.66	J/mol×K	1050.25	Joback Method
cpg	1234.58	J/mol×K	1241.03	Joback Method
dvisc	0.0000348	Pa×s	1012.09	Joback Method

dvisc	0.0000441	Pa×s	943.59	Joback Method
dvisc	0.0000579	Pa×s	875.10	Joback Method
dvisc	0.0000796	Pa×s	806.60	Joback Method
dvisc	0.0001162	Pa×s	738.10	Joback Method
dvisc	0.0001831	Pa×s	669.61	Joback Method
dvisc	0.0003203	Pa×s	601.11	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=U382655&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