1,2-Cyclohexanedicarboxylic acid, 4-chloro-2-methylphenyl decyl ester

Inchi: InChI=1S/C25H37ClO4/c1-3-4-5-6-7-8-9-12-17-29-24(27)21-13-10-11-14-22(21)25(28)30

InchiKey: BZXDWFAIPYSKAS-UHFFFAOYSA-N

Formula: C25H37ClO4

SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 437.01

Physical Properties

Property code	Value	Unit	Source
gf	-210.26	kJ/mol	Joback Method
hf	-817.10	kJ/mol	Joback Method
hfus	56.45	kJ/mol	Joback Method
hvap	97.66	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	7.044		Crippen Method
mcvol	355.610	ml/mol	McGowan Method
pc	1047.33	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook
tb	1012.93	K	Joback Method
tc	1241.69	K	Joback Method
tf	600.35	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1205.06	J/mol×K	1012.93	Joback Method
cpg	1262.43	J/mol×K	1203.56	Joback Method
cpg	1254.44	J/mol×K	1165.43	Joback Method
cpg	1244.74	J/mol×K	1127.31	Joback Method
cpg	1233.31	J/mol×K	1089.18	Joback Method
cpg	1220.09	J/mol×K	1051.06	Joback Method
cpg	1268.78	J/mol×K	1241.69	Joback Method
dvisc	0.0000317	Pa×s	1012.93	Joback Method

dvisc	0.0000404	Pa×s	944.17	Joback Method
dvisc	0.0000535	Pa×s	875.40	Joback Method
dvisc	0.0000743	Pa×s	806.64	Joback Method
dvisc	0.0001098	Pa×s	737.88	Joback Method
dvisc	0.0001759	Pa×s	669.11	Joback Method
dvisc	0.0003136	Pa×s	600.35	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=U339793&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

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