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

Inchi: InChI=1S/C29H43ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-16-21-33-28(31)25-17-14-15-18-26

InchiKey: VPETZAJLOSQPPE-UHFFFAOYSA-N

Formula: C29H43ClO4

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

Mol. weight [g/mol]: 491.10

Physical Properties

Property code	Value	Unit	Source
gf	-146.62	kJ/mol	Joback Method
hf	-841.88	kJ/mol	Joback Method
hfus	68.03	kJ/mol	Joback Method
hvap	106.86	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.381		Crippen Method
mcvol	407.670	ml/mol	McGowan Method
pc	846.03	kPa	Joback Method
rinpol	3528.00		NIST Webbook
rinpol	3528.00		NIST Webbook
tb	1103.61	K	Joback Method
tc	1353.75	K	Joback Method
tf	646.19	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1419.65	J/mol×K	1103.61	Joback Method
cpg	1433.83	J/mol×K	1145.30	Joback Method
cpg	1445.86	J/mol×K	1186.99	Joback Method
cpg	1455.82	J/mol×K	1228.68	Joback Method
cpg	1463.78	J/mol×K	1270.37	Joback Method
cpg	1469.82	J/mol×K	1312.06	Joback Method
cpg	1474.02	J/mol×K	1353.75	Joback Method
dvisc	0.0001996	Pa×s	646.19	Joback Method

dvisc	0.0001098	Pa×s	722.43	Joback Method
dvisc	0.0000677	Pa×s	798.66	Joback Method
dvisc	0.0000454	Pa×s	874.90	Joback Method
dvisc	0.0000325	Pa×s	951.14	Joback Method
dvisc	0.0000244	Pa×s	1027.37	Joback Method
dvisc	0.0000191	Pa×s	1103.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382658&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