

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

Inchi:	InChI=1S/C28H41ClO4/c1-3-4-5-6-7-8-9-10-11-12-15-20-32-27(30)24-16-13-14-17-25(26)
InchiKey:	SKNFMLFECCEQPN-UHFFFAOYSA-N
Formula:	C28H41ClO4
SMILES:	CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	477.08

Physical Properties

Property code	Value	Unit	Source
gf	-155.04	kJ/mol	Joback Method
hf	-821.24	kJ/mol	Joback Method
hfus	65.44	kJ/mol	Joback Method
hvap	104.63	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	7.990		Crippen Method
mvol	393.580	ml/mol	McGowan Method
pc	895.34	kPa	Joback Method
rinpol	3422.00		NIST Webbook
rinpol	3422.00		NIST Webbook
tb	1080.73	K	Joback Method
tc	1323.82	K	Joback Method
tf	634.92	K	Joback Method
vc	1.510	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1357.68	J/molxK	1080.73	Joback Method
cpg	1371.92	J/molxK	1121.25	Joback Method
cpg	1384.14	J/molxK	1161.76	Joback Method
cpg	1394.39	J/molxK	1202.28	Joback Method
cpg	1402.76	J/molxK	1242.79	Joback Method
cpg	1409.29	J/molxK	1283.31	Joback Method
cpg	1414.07	J/molxK	1323.82	Joback Method
dvisc	0.0002255	Paxs	634.92	Joback Method

dvisc	0.0001252	Paxs	709.22	Joback Method
dvisc	0.0000777	Paxs	783.52	Joback Method
dvisc	0.0000524	Paxs	857.83	Joback Method
dvisc	0.0000376	Paxs	932.13	Joback Method
dvisc	0.0000284	Paxs	1006.43	Joback Method
dvisc	0.0000222	Paxs	1080.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382657&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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