

1,2-Cyclohexanedicarboxylic acid, 3-chlorophenyl undecyl ester

Inchi:	InChI=1S/C25H37ClO4/c1-2-3-4-5-6-7-8-9-12-18-29-24(27)22-16-10-11-17-23(22)25(28)
InchiKey:	LHSLHQBIMNKLCQ-UHFFFAOYSA-N
Formula:	C25H37ClO4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	437.01

Physical Properties

Property code	Value	Unit	Source
gf	-200.63	kJ/mol	Joback Method
hf	-805.63	kJ/mol	Joback Method
hfus	56.83	kJ/mol	Joback Method
hvap	97.00	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	7.126		Crippen Method
mvol	355.610	ml/mol	McGowan Method
pc	1057.57	kPa	Joback Method
rinpol	3153.00		NIST Webbook
rinpol	3153.00		NIST Webbook
tb	1007.95	K	Joback Method
tc	1235.71	K	Joback Method
tf	587.83	K	Joback Method
vc	1.357	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.00	J/molxK	1007.95	Joback Method
cpg	1221.24	J/molxK	1045.91	Joback Method
cpg	1234.69	J/molxK	1083.87	Joback Method
cpg	1246.42	J/molxK	1121.83	Joback Method
cpg	1256.46	J/molxK	1159.79	Joback Method
cpg	1264.88	J/molxK	1197.75	Joback Method
cpg	1271.71	J/molxK	1235.71	Joback Method
dvisc	0.0003512	Paxs	587.83	Joback Method

dvisc	0.0001887	Paxs	657.85	Joback Method
dvisc	0.0001142	Paxs	727.87	Joback Method
dvisc	0.0000755	Paxs	797.89	Joback Method
dvisc	0.0000534	Paxs	867.91	Joback Method
dvisc	0.0000397	Paxs	937.93	Joback Method
dvisc	0.0000308	Paxs	1007.95	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=U339695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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