

Isophthalic acid, 4-chlorophenyl undecyl ester

Inchi:	InChI=1S/C25H31ClO4/c1-2-3-4-5-6-7-8-9-10-18-29-24(27)20-12-11-13-21(19-20)25(28)
InchiKey:	ANDOPGRMPDEQLT-UHFFFAOYSA-N
Formula:	C25H31ClO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2)c1
Mol. weight [g/mol]:	430.96

Physical Properties

Property code	Value	Unit	Source
gf	-114.59	kJ/mol	Joback Method
hf	-614.55	kJ/mol	Joback Method
hfus	57.58	kJ/mol	Joback Method
hvap	99.82	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	7.247		Crippen Method
mvol	342.710	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	3435.00		NIST Webbook
rinpol	3435.00		NIST Webbook
tb	1024.73	K	Joback Method
tc	1256.61	K	Joback Method
tf	623.63	K	Joback Method
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.41	J/molxK	1024.73	Joback Method
cpg	1111.44	J/molxK	1063.38	Joback Method
cpg	1123.01	J/molxK	1102.02	Joback Method
cpg	1133.19	J/molxK	1140.67	Joback Method
cpg	1142.03	J/molxK	1179.31	Joback Method
cpg	1149.60	J/molxK	1217.96	Joback Method
cpg	1155.94	J/molxK	1256.61	Joback Method
dvisc	0.0002187	Paxs	623.63	Joback Method

dvisc	0.0001263	Paxs	690.48	Joback Method
dvisc	0.0000804	Paxs	757.33	Joback Method
dvisc	0.0000550	Paxs	824.18	Joback Method
dvisc	0.0000399	Paxs	891.03	Joback Method
dvisc	0.0000302	Paxs	957.88	Joback Method
dvisc	0.0000238	Paxs	1024.73	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=U344585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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