Phthalic acid, 2-(4-chlorophenyl)ethyl undecyl ester

Inchi: InChI=1S/C27H35ClO4/c1-2-3-4-5-6-7-8-9-12-20-31-26(29)24-13-10-11-14-25(24)27(30)
InchiKey: BVIVXNJUUWYZEC-UHFFFAOYSA-N
Formula: C27H35ClO4
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccc(Cl)cc1
Mol. weight [g/mol]: 459.02

Physical Properties

Property code	Value	Unit	Source
gf	-97.75	kJ/mol	Joback Method
hf	-655.83	kJ/mol	Joback Method
hfus	62.76	kJ/mol	Joback Method
hvap	104.27	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	7.427		Crippen Method
mcvol	370.890	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	3402.00		NIST Webbook
rinpol	3402.00		NIST Webbook
tb	1070.49	K	Joback Method
tc	1310.58	K	Joback Method
tf	646.17	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1219.77	J/mol×K	1070.49	Joback Method
cpg	1232.96	J/mol×K	1110.51	Joback Method
cpg	1244.58	J/mol×K	1150.52	Joback Method
cpg	1254.69	J/mol×K	1190.54	Joback Method
cpg	1263.38	J/mol×K	1230.55	Joback Method
cpg	1270.70	J/mol×K	1270.57	Joback Method
cpg	1276.75	J/mol×K	1310.58	Joback Method
dvisc	0.0001718	Pa×s	646.17	Joback Method

dvisc	0.0000973	Pa×s	716.89	Joback Method
dvisc	0.0000610	Pa×s	787.61	Joback Method
dvisc	0.0000413	Pa×s	858.33	Joback Method
dvisc	0.0000297	Pa×s	929.05	Joback Method
dvisc	0.0000224	Pa×s	999.77	Joback Method
dvisc	0.0000175	Pa×s	1070.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377845&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