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

Inchi: InChI=1S/C27H35ClO5/c1-2-3-4-5-6-7-8-9-14-19-32-26(29)22-15-10-11-16-23(22)27(30)
InchiKey: RCCXEIBYZFYFRH-UHFFFAOYSA-N
Formula: C27H35ClO5
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccccc1Cl
Mol. weight [g/mol]: 475.02

Physical Properties

Property code	Value	Unit	Source
gf	-202.75	kJ/mol	Joback Method
hf	-788.05	kJ/mol	Joback Method
hfus	63.95	kJ/mol	Joback Method
hvap	106.68	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	7.263		Crippen Method
mcvol	376.760	ml/mol	McGowan Method
pc	1014.24	kPa	Joback Method
rinpol	3480.00		NIST Webbook
rinpol	3480.00		NIST Webbook
tb	1092.91	K	Joback Method
tc	1338.57	K	Joback Method
tf	668.40	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.83	J/mol×K	1092.91	Joback Method
cpg	1256.59	J/mol×K	1133.85	Joback Method
cpg	1266.49	J/mol×K	1174.80	Joback Method
cpg	1274.58	J/mol×K	1215.74	Joback Method
cpg	1280.93	J/mol×K	1256.68	Joback Method
cpg	1285.59	J/mol×K	1297.62	Joback Method
cpg	1288.62	J/mol×K	1338.57	Joback Method
dvisc	0.0001198	Pa×s	668.40	Joback Method

dvisc	0.0000690	Pa×s	739.15	Joback Method
dvisc	0.0000438	Pa×s	809.90	Joback Method
dvisc	0.0000299	Pa×s	880.65	Joback Method
dvisc	0.0000216	Pa×s	951.41	Joback Method
dvisc	0.0000163	Pa×s	1022.16	Joback Method
dvisc	0.0000128	Pa×s	1092.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377912&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