Phthalic acid, 3,4,5-trichlorophenyl undecyl ester

Inchi: InChI=1S/C25H29Cl3O4/c1-2-3-4-5-6-7-8-9-12-15-31-24(29)19-13-10-11-14-20(19)25(30
InchiKey: AMSLLOFJQNIXMT-UHFFFAOYSA-N
Formula: C25H29Cl3O4
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]: 499.85

Physical Properties

Property code	Value	Unit	Source
gf	-157.71	kJ/mol	Joback Method
hf	-668.97	kJ/mol	Joback Method
hfus	65.20	kJ/mol	Joback Method
hvap	109.91	kJ/mol	Joback Method
log10ws	-10.04		Crippen Method
logp	8.554		Crippen Method
mcvol	367.190	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	3487.00		NIST Webbook
rinpol	3487.00		NIST Webbook
tb	1109.55	K	Joback Method
tc	1358.42	K	Joback Method
tf	708.51	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.94	J/mol×K	1109.55	Joback Method
cpg	1143.84	J/mol×K	1151.03	Joback Method
cpg	1152.17	J/mol×K	1192.51	Joback Method
cpg	1158.97	J/mol×K	1233.98	Joback Method
cpg	1164.32	J/mol×K	1275.46	Joback Method
cpg	1168.26	J/mol×K	1316.94	Joback Method
cpg	1170.85	J/mol×K	1358.42	Joback Method
dvisc	0.0001210	Pa×s	708.51	Joback Method

dvisc	0.0000764	Pa×s	775.35	Joback Method
dvisc	0.0000519	Pa×s	842.19	Joback Method
dvisc	0.0000373	Pa×s	909.03	Joback Method
dvisc	0.0000281	Pa×s	975.87	Joback Method
dvisc	0.0000219	Pa×s	1042.71	Joback Method
dvisc	0.0000176	Pa×s	1109.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357074&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

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