Phthalic acid, 4-chloro-2-methylphenyl undecyl ester

Inchi: InChI=1S/C26H33ClO4/c1-3-4-5-6-7-8-9-10-13-18-30-25(28)22-14-11-12-15-23(22)26(29

InchiKey: UDBLMMCZIPWHMC-UHFFFAOYSA-N

Formula: C26H33ClO4

SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 444.99

Physical Properties

Property code	Value	Unit	Source
gf	-115.80	kJ/mol	Joback Method
hf	-646.66	kJ/mol	Joback Method
hfus	59.78	kJ/mol	Joback Method
hvap	102.70	kJ/mol	Joback Method
log10ws	-9.15		Crippen Method
logp	7.555		Crippen Method
mcvol	356.800	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	3226.00		NIST Webbook
rinpol	3226.00		NIST Webbook
tb	1052.59	K	Joback Method
tc	1289.08	K	Joback Method
tf	647.42	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.57	J/mol×K	1052.59	Joback Method
cpg	1170.47	J/mol×K	1092.01	Joback Method
cpg	1181.81	J/mol×K	1131.42	Joback Method
cpg	1191.65	J/mol×K	1170.84	Joback Method
cpg	1200.03	J/mol×K	1210.25	Joback Method
cpg	1207.03	J/mol×K	1249.67	Joback Method
cpg	1212.70	J/mol×K	1289.08	Joback Method
dvisc	0.0001764	Pa×s	647.42	Joback Method

dvisc	0.0001046	Pa×s	714.95	Joback Method
dvisc	0.0000679	Pa×s	782.48	Joback Method
dvisc	0.0000472	Pa×s	850.00	Joback Method
dvisc	0.0000346	Pa×s	917.53	Joback Method
dvisc	0.0000265	Pa×s	985.06	Joback Method
dvisc	0.0000210	Pa×s	1052.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356383&Units=SI

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