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

Inchi: InChI=1S/C27H35ClO4/c1-3-4-5-6-7-8-9-10-11-14-19-31-26(29)23-15-12-13-16-24(23)27

InchiKey: BUABLNGWBIWGDH-UHFFFAOYSA-N

Formula: C27H35ClO4

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

Mol. weight [g/mol]: 459.02

Physical Properties

Property code	Value	Unit	Source
gf	-107.38	kJ/mol	Joback Method
hf	-667.30	kJ/mol	Joback Method
hfus	62.37	kJ/mol	Joback Method
hvap	104.93	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	7.945		Crippen Method
mcvol	370.890	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	3333.00		NIST Webbook
rinpol	3333.00		NIST Webbook
tb	1075.47	K	Joback Method
tc	1316.69	K	Joback Method
tf	658.69	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.40	J/mol×K	1075.47	Joback Method
cpg	1231.36	J/mol×K	1115.67	Joback Method
cpg	1242.68	J/mol×K	1155.88	Joback Method
cpg	1252.44	J/mol×K	1196.08	Joback Method
cpg	1260.69	J/mol×K	1236.28	Joback Method
cpg	1267.50	J/mol×K	1276.48	Joback Method
cpg	1272.94	J/mol×K	1316.69	Joback Method
dvisc	0.0001565	Pa×s	658.69	Joback Method

dvisc	0.0000919	Pa×s	728.15	Joback Method
dvisc	0.0000592	Pa×s	797.62	Joback Method
dvisc	0.0000410	Pa×s	867.08	Joback Method
dvisc	0.0000299	Pa×s	936.54	Joback Method
dvisc	0.0000228	Pa×s	1006.01	Joback Method
dvisc	0.0000180	Pa×s	1075.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356382&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