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

Inchi: InChI=1S/C28H37ClO4/c1-3-4-5-6-7-8-9-10-11-12-15-20-32-27(30)24-16-13-14-17-25(24

InchiKey: SXRPBUATCBSGFC-UHFFFAOYSA-N

Formula: C28H37ClO4

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

Mol. weight [g/mol]: 473.04

Physical Properties

Property code	Value	Unit	Source
gf	-98.96	kJ/mol	Joback Method
hf	-687.94	kJ/mol	Joback Method
hfus	64.96	kJ/mol	Joback Method
hvap	107.16	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	8.335		Crippen Method
mcvol	384.980	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpol	3440.00		NIST Webbook
rinpol	3440.00		NIST Webbook
tb	1098.35	K	Joback Method
tc	1345.45	K	Joback Method
tf	669.96	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1279.55	J/mol×K	1098.35	Joback Method
cpg	1292.59	J/mol×K	1139.53	Joback Method
cpg	1303.90	J/mol×K	1180.72	Joback Method
cpg	1313.56	J/mol×K	1221.90	Joback Method
cpg	1321.66	J/mol×K	1263.08	Joback Method
cpg	1328.26	J/mol×K	1304.27	Joback Method
cpg	1333.43	J/mol×K	1345.45	Joback Method
dvisc	0.0001385	Pa×s	669.96	Joback Method

dvisc	0.0000806	Pa×s	741.36	Joback Method
dvisc	0.0000516	Pa×s	812.76	Joback Method
dvisc	0.0000355	Pa×s	884.16	Joback Method
dvisc	0.0000258	Pa×s	955.55	Joback Method
dvisc	0.0000196	Pa×s	1026.95	Joback Method
dvisc	0.0000154	Pa×s	1098.35	Joback Method

Sources

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=U356381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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