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

Inchi: InChI=1S/C28H37ClO5/c1-2-3-4-5-6-7-8-9-10-15-20-33-27(30)23-16-11-12-17-24(23)28(

InchiKey: DRSYKUNOMKGZLP-UHFFFAOYSA-N

Formula: C28H37ClO5

SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccccc1Cl

Mol. weight [g/mol]: 489.04

Physical Properties

Property code	Value	Unit	Source
gf	-194.33	kJ/mol	Joback Method
hf	-808.69	kJ/mol	Joback Method
hfus	66.54	kJ/mol	Joback Method
hvap	108.91	kJ/mol	Joback Method
log10ws	-9.02		Crippen Method
logp	7.653		Crippen Method
mcvol	390.850	ml/mol	McGowan Method
pc	954.96	kPa	Joback Method
rinpol	3580.00		NIST Webbook
rinpol	3580.00		NIST Webbook
tb	1115.79	K	Joback Method
tc	1368.33	K	Joback Method
tf	679.67	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1305.53	J/mol×K	1115.79	Joback Method
cpg	1317.25	J/mol×K	1157.88	Joback Method
cpg	1326.99	J/mol×K	1199.97	Joback Method
cpg	1334.82	J/mol×K	1242.06	Joback Method
cpg	1340.81	J/mol×K	1284.15	Joback Method
cpg	1345.03	J/mol×K	1326.24	Joback Method
cpg	1347.54	J/mol×K	1368.33	Joback Method
dvisc	0.0001055	Pa×s	679.67	Joback Method

dvisc	0.0000602	Pa×s	752.36	Joback Method
dvisc	0.0000380	Pa×s	825.04	Joback Method
dvisc	0.0000258	Pa×s	897.73	Joback Method
dvisc	0.0000186	Pa×s	970.42	Joback Method
dvisc	0.0000140	Pa×s	1043.10	Joback Method
dvisc	0.0000109	Pa×s	1115.79	Joback Method

Sources

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=U377913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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