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

Inchi: InChI=1S/C29H39ClO5/c1-2-3-4-5-6-7-8-9-10-11-16-21-34-28(31)24-17-12-13-18-25(24)

InchiKey: PQYKVGSVGAKUBW-UHFFFAOYSA-N

Formula: C29H39ClO5

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

Mol. weight [g/mol]: 503.07

Physical Properties

Property code	Value	Unit	Source
gf	-185.91	kJ/mol	Joback Method
hf	-829.33	kJ/mol	Joback Method
hfus	69.13	kJ/mol	Joback Method
hvap	111.13	kJ/mol	Joback Method
log10ws	-9.43		Crippen Method
logp	8.044		Crippen Method
mcvol	404.940	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	3681.00		NIST Webbook
tb	1138.67	K	Joback Method
tc	1399.41	K	Joback Method
tf	690.94	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1366.45	J/mol×K	1138.67	Joback Method
cpg	1378.13	J/mol×K	1182.13	Joback Method
cpg	1387.70	J/mol×K	1225.58	Joback Method
cpg	1395.23	J/mol×K	1269.04	Joback Method
cpg	1400.82	J/mol×K	1312.49	Joback Method
cpg	1404.53	J/mol×K	1355.95	Joback Method
cpg	1406.45	J/mol×K	1399.41	Joback Method
dvisc	0.0000927	Pa×s	690.94	Joback Method
dvisc	0.0000525	Pa×s	765.56	Joback Method

dvisc	0.0000329	Pa×s	840.18	Joback Method
dvisc	0.0000222	Pa×s	914.81	Joback Method
dvisc	0.0000159	Pa×s	989.43	Joback Method
dvisc	0.0000120	Pa×s	1064.05	Joback Method
dvisc	0.0000093	Pa×s	1138.67	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=U377914&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