Phthalic acid, 2-(4-chlorophenyl)ethyl nonyl ester

Inchi: InChI=1S/C25H31ClO4/c1-2-3-4-5-6-7-10-18-29-24(27)22-11-8-9-12-23(22)25(28)30-19-

InchiKey: KDIWRDPYKNIJCS-UHFFFAOYSA-N

Formula: C25H31ClO4

SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccc(Cl)cc1

Mol. weight [g/mol]: 430.96

Physical Properties

Property code	Value	Unit	Source
gf	-114.59	kJ/mol	Joback Method
hf	-614.55	kJ/mol	Joback Method
hfus	57.58	kJ/mol	Joback Method
hvap	99.82	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	6.647		Crippen Method
mcvol	342.710	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	3202.00		NIST Webbook
rinpol	3202.00		NIST Webbook
tb	1024.73	K	Joback Method
tc	1256.61	K	Joback Method
tf	623.63	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.41	J/mol×K	1024.73	Joback Method
cpg	1111.44	J/mol×K	1063.38	Joback Method
cpg	1123.01	J/mol×K	1102.02	Joback Method
cpg	1133.19	J/mol×K	1140.67	Joback Method
cpg	1142.03	J/mol×K	1179.31	Joback Method
cpg	1149.60	J/mol×K	1217.96	Joback Method
cpg	1155.94	J/mol×K	1256.61	Joback Method
dvisc	0.0002187	Pa×s	623.63	Joback Method

dvisc	0.0001263	Pa×s	690.48	Joback Method
dvisc	0.0000804	Pa×s	757.33	Joback Method
dvisc	0.0000550	Pa×s	824.18	Joback Method
dvisc	0.0000399	Pa×s	891.03	Joback Method
dvisc	0.0000302	Pa×s	957.88	Joback Method
dvisc	0.0000238	Pa×s	1024.73	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=U377843&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

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