

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

Inchi:	InChI=1S/C31H43ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-24-35-30(33)28-17-14-15-18
InchiKey:	AGZGPZKZAHDPCU-UHFFFAOYSA-N
Formula:	C31H43ClO4
SMILES:	CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccc(Cl)cc1
Mol. weight [g/mol]:	515.12

Physical Properties

Property code	Value	Unit	Source
gf	-64.07	kJ/mol	Joback Method
hf	-738.39	kJ/mol	Joback Method
hfus	73.12	kJ/mol	Joback Method
hvap	113.17	kJ/mol	Joback Method
log10ws	-10.54		Crippen Method
logp	8.988		Crippen Method
mvol	427.250	ml/mol	McGowan Method
pc	813.07	kPa	Joback Method
rinpol	3804.00		NIST Webbook
rinpol	3804.00		NIST Webbook
tb	1162.01	K	Joback Method
tc	1433.00	K	Joback Method
tf	691.25	K	Joback Method
vc	1.653	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1466.43	J/molxK	1162.01	Joback Method
cpg	1480.20	J/molxK	1207.18	Joback Method
cpg	1492.00	J/molxK	1252.34	Joback Method
cpg	1501.97	J/molxK	1297.51	Joback Method
cpg	1510.24	J/molxK	1342.67	Joback Method
cpg	1516.94	J/molxK	1387.84	Joback Method
cpg	1522.21	J/molxK	1433.00	Joback Method
dvisc	0.0001030	Paxs	691.25	Joback Method

dvisc	0.0000562	Paxs	769.71	Joback Method
dvisc	0.0000344	Paxs	848.17	Joback Method
dvisc	0.0000228	Paxs	926.63	Joback Method
dvisc	0.0000161	Paxs	1005.09	Joback Method
dvisc	0.0000120	Paxs	1083.55	Joback Method
dvisc	0.0000093	Paxs	1162.01	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=U377849&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

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