

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

Inchi:	InChI=1S/C30H41ClO5/c1-2-3-4-5-6-7-8-9-10-11-12-17-22-35-29(32)25-18-13-14-19-26
InchiKey:	XGWCHRUPKHHRFP-UHFFFAOYSA-N
Formula:	C30H41ClO5
SMILES:	CCCCCCCCCCCCCOC(=O)c1cccc1C(=O)OCCOc1cccc1Cl
Mol. weight [g/mol]:	517.10

Physical Properties

Property code	Value	Unit	Source
gf	-177.49	kJ/mol	Joback Method
hf	-849.97	kJ/mol	Joback Method
hfus	71.72	kJ/mol	Joback Method
hvap	113.36	kJ/mol	Joback Method
log10ws	-9.85		Crippen Method
logp	8.434		Crippen Method
mcvol	419.030	ml/mol	McGowan Method
pc	850.98	kPa	Joback Method
rinpol	3786.00		NIST Webbook
rinpol	3786.00		NIST Webbook
tb	1161.55	K	Joback Method
tc	1431.87	K	Joback Method
tf	702.21	K	Joback Method
vc	1.615	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1427.56	J/molxK	1161.55	Joback Method
cpg	1464.02	J/molxK	1386.82	Joback Method
cpg	1460.88	J/molxK	1341.76	Joback Method
cpg	1455.76	J/molxK	1296.71	Joback Method
cpg	1448.56	J/molxK	1251.66	Joback Method
cpg	1439.19	J/molxK	1206.60	Joback Method
cpg	1465.28	J/molxK	1431.87	Joback Method
dvisc	0.0000079	Paxs	1161.55	Joback Method

dvisc	0.0000102	Paxs	1084.99	Joback Method
dvisc	0.0000136	Paxs	1008.44	Joback Method
dvisc	0.0000191	Paxs	931.88	Joback Method
dvisc	0.0000284	Paxs	855.32	Joback Method
dvisc	0.0000456	Paxs	778.77	Joback Method
dvisc	0.0000813	Paxs	702.21	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=U377915&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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