

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

Inchi:	InChI=1S/C25H31ClO5/c1-2-3-4-5-6-7-12-17-30-24(27)20-13-8-9-14-21(20)25(28)31-19
InchiKey:	OBSWCRQOWUSOBY-UHFFFAOYSA-N
Formula:	C25H31ClO5
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccccc1Cl
Mol. weight [g/mol]:	446.96

Physical Properties

Property code	Value	Unit	Source
gf	-219.59	kJ/mol	Joback Method
hf	-746.77	kJ/mol	Joback Method
hfus	58.77	kJ/mol	Joback Method
hvap	102.23	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.483		Crippen Method
mcvol	348.580	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	3284.00		NIST Webbook
tb	1047.15	K	Joback Method
tc	1282.61	K	Joback Method
tf	645.86	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.26	J/molxK	1047.15	Joback Method
cpg	1167.08	J/molxK	1243.37	Joback Method
cpg	1161.70	J/molxK	1204.13	Joback Method
cpg	1154.76	J/molxK	1164.88	Joback Method
cpg	1146.24	J/molxK	1125.64	Joback Method
cpg	1136.09	J/molxK	1086.39	Joback Method
cpg	1170.96	J/molxK	1282.61	Joback Method
dvisc	0.0000175	Paxs	1047.15	Joback Method
dvisc	0.0000222	Paxs	980.27	Joback Method

dvisc	0.0000292	Paxs	913.39	Joback Method
dvisc	0.0000400	Paxs	846.51	Joback Method
dvisc	0.0000580	Paxs	779.62	Joback Method
dvisc	0.0000900	Paxs	712.74	Joback Method
dvisc	0.0001532	Paxs	645.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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