

Di-[2-(4-tert-butyl-2,6-dichlorophenoxy) ethyl] ether

Inchi:	InChI=1S/C24H30Cl4O3/c1-23(2,3)15-11-17(25)21(18(26)12-15)30-9-7-29-8-10-31-22-1
InchiKey:	NZBZIWD0AAFPSW-UHFFFAOYSA-N
Formula:	C24H30Cl4O3
SMILES:	CC(C)(C)c1cc(Cl)c(OCCOCCOc2c(Cl)cc(C(C)(C)C)cc2Cl)c(Cl)c1
Mol. weight [g/mol]:	508.31
CAS:	116401-27-5

Physical Properties

Property code	Value	Unit	Source
gf	-38.80	kJ/mol	Joback Method
hf	-611.57	kJ/mol	Joback Method
hfus	49.19	kJ/mol	Joback Method
hvap	99.72	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	8.370		Crippen Method
mcvol	368.070	ml/mol	McGowan Method
pc	1033.24	kPa	Joback Method
tb	1042.28	K	Joback Method
tc	1283.59	K	Joback Method
tf	679.41	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.32	J/molxK	1042.28	Joback Method
cpg	1120.76	J/molxK	1082.50	Joback Method
cpg	1131.85	J/molxK	1122.72	Joback Method
cpg	1141.69	J/molxK	1162.94	Joback Method
cpg	1150.34	J/molxK	1203.15	Joback Method
cpg	1157.89	J/molxK	1243.37	Joback Method
cpg	1164.39	J/molxK	1283.59	Joback Method
dvisc	0.0000608	Paxs	679.41	Joback Method
dvisc	0.0000382	Paxs	739.89	Joback Method

dvisc	0.0000257	Paxs	800.37	Joback Method
dvisc	0.0000183	Paxs	860.85	Joback Method
dvisc	0.0000137	Paxs	921.32	Joback Method
dvisc	0.0000106	Paxs	981.80	Joback Method
dvisc	0.0000084	Paxs	1042.28	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=C116401275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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