

2-(2,4-Ditert-butyl-6-chlorophenoxy)ethanol

Inchi:	InChI=1S/C16H25ClO2/c1-15(2,3)11-9-12(16(4,5)6)14(13(17)10-11)19-8-7-18/h9-10,18H
InchiKey:	SRZIOMHHMBGULK-UHFFFAOYSA-N
Formula:	C16H25ClO2
SMILES:	CC(C)(C)c1cc(Cl)c(OCCO)c(C(C)(C)C)c1
Mol. weight [g/mol]:	284.82
CAS:	116401-36-6

Physical Properties

Property code	Value	Unit	Source
gf	-80.71	kJ/mol	Joback Method
hf	-489.14	kJ/mol	Joback Method
hfus	24.72	kJ/mol	Joback Method
hvap	76.35	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.306		Crippen Method
mcvol	236.520	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
tb	752.67	K	Joback Method
tc	955.98	K	Joback Method
tf	451.87	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.36	J/molxK	752.67	Joback Method
cpg	741.39	J/molxK	922.10	Joback Method
cpg	729.79	J/molxK	888.21	Joback Method
cpg	717.45	J/molxK	854.33	Joback Method
cpg	704.30	J/molxK	820.44	Joback Method
cpg	690.28	J/molxK	786.56	Joback Method
cpg	752.29	J/molxK	955.98	Joback Method
dvisc	0.0000152	Paxs	752.67	Joback Method
dvisc	0.0000226	Paxs	702.54	Joback Method

dvisc	0.0000358	Paxs	652.40	Joback Method
dvisc	0.0000611	Paxs	602.27	Joback Method
dvisc	0.0001149	Paxs	552.14	Joback Method
dvisc	0.0002453	Paxs	502.00	Joback Method
dvisc	0.0006193	Paxs	451.87	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=C116401366&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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