Ethanol, 2-[4-(1,1-dimethylethyl)phenoxy]-

Other names: Ethanol, 2-(p-tert-butylphenoxy)-
2-(p-tert-Butylphenoxy)ethanol
2-(p-tert-Butylphenyloxy)ethanol
«beta»-(p-tert-Butylphenoxy)ethanol
2-(4-tert-Butylphenoxy)ethanol
2-(4-(1,1-Dimethylethyl)phenoxyl)ethanol

Inchi: InChI=1S/C12H18O2/c1-12(2,3)10-4-6-11(7-5-10)14-9-8-13/h4-7,13H,8-9H2,1-3H3

InchiKey: KGPFHDDLZCYWAO-UHFFFAOYSA-N

Formula: C12H18O2

SMILES: CC(C)(C)c1ccc(OCCO)cc1

Mol. weight [g/mol]: 194.27

CAS: 713-46-2

Physical Properties

Property code	Value	Unit	Source
gf	-86.04	kJ/mol	Joback Method
hf	-359.15	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	63.04	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.355		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1519.90		NIST Webbook
tb	616.99	K	Joback Method
tc	814.44	K	Joback Method
tf	349.41	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.50	J/mol×K	616.99	Joback Method
cpg	449.54	J/mol×K	649.90	Joback Method

cpg	462.77	J/mol×K	682.81	Joback Method
cpg	475.22	J/mol×K	715.72	Joback Method
cpg	486.93	J/mol×K	748.62	Joback Method
cpg	497.93	J/mol×K	781.53	Joback Method
cpg	508.26	J/mol×K	814.44	Joback Method
dvisc	0.0037828	Pa×s	349.41	Joback Method
dvisc	0.0012155	Pa×s	394.01	Joback Method
dvisc	0.0004920	Pa×s	438.60	Joback Method
dvisc	0.0002353	Pa×s	483.20	Joback Method
dvisc	0.0001275	Pa×s	527.80	Joback Method
dvisc	0.0000760	Pa×s	572.39	Joback Method
dvisc	0.0000488	Pa×s	616.99	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C713462&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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