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

Other names: Ethanol, 2-(p-tert-pentylphenoxy)-
2-(p-tert-Amylphenoxy)ethanol
2-(p-tert-Pentylphenoxy)ethanol
p-t-Amylphenoxyethanol
Ethanol, 2-[p-(1,1-dimethylpropyl)phenoxy]-
2-[4-(1,1-dimethylpropyl)phenoxy]ethanol
Inchi: InChI=1S/C13H20O2/c1-4-13(2,3)11-5-7-12(8-6-11)15-10-9-14/h5-8,14H,4,9-10H2,1-3H
InchiKey: BXXDXUTVAFRBKC-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CCC(C)(C)c1ccc(OCCO)cc1
Mol. weight [g/mol]: 208.30
CAS: 6382-07-6

Physical Properties

Property code	Value	Unit	Source
gf	-77.62	kJ/mol	Joback Method
hf	-379.79	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	65.26	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.745		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
tb	639.87	K	Joback Method
tc	834.90	K	Joback Method
tf	360.68	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.07	J/mol×K	639.87	Joback Method
cpg	500.65	J/mol×K	672.37	Joback Method
cpg	514.40	J/mol×K	704.88	Joback Method

cpg	527.35	J/mol×K	737.38	Joback Method
cpg	539.53	J/mol×K	769.89	Joback Method
cpg	551.00	J/mol×K	802.39	Joback Method
cpg	561.77	J/mol×K	834.90	Joback Method
dvisc	0.0031545	Pa×s	360.68	Joback Method
dvisc	0.0010087	Pa×s	407.21	Joback Method
dvisc	0.0004075	Pa×s	453.74	Joback Method
dvisc	0.0001949	Pa×s	500.27	Joback Method
dvisc	0.0001057	Pa×s	546.81	Joback Method
dvisc	0.0000631	Pa×s	593.34	Joback Method
dvisc	0.0000406	Pa×s	639.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6382076&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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