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

Other names: 2-(p-sec-Butylphenoxy)ethanol
2-(4-sec-butylphenoxy)ethanol
Inchi: InChI=1S/C12H18O2/c1-3-10(2)11-4-6-12(7-5-11)14-9-8-13/h4-7,10,13H,3,8-9H2,1-2H3
InchiKey: XMPKZDNQLSEWRU-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CCC(C)c1ccc(OCCO)cc1
Mol. weight [g/mol]: 194.27
CAS: 5349-63-3

Physical Properties

Property code	Value	Unit	Source
gf	-91.32	kJ/mol	Joback Method
hf	-355.68	kJ/mol	Joback Method
hfus	22.24	kJ/mol	Joback Method
hvap	63.95	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.571		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	619.78	K	Joback Method
tc	810.79	K	Joback Method
tf	331.99	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.72	J/mol×K	619.78	Joback Method
cpg	446.46	J/mol×K	651.62	Joback Method
cpg	459.49	J/mol×K	683.45	Joback Method
cpg	471.84	J/mol×K	715.29	Joback Method
cpg	483.53	J/mol×K	747.12	Joback Method

cpg	494.56	J/mol×K	778.96	Joback Method
cpg	504.95	J/mol×K	810.79	Joback Method
dvisc	0.0051871	Pa×s	331.99	Joback Method
dvisc	0.0014778	Pa×s	379.95	Joback Method
dvisc	0.0005579	Pa×s	427.92	Joback Method
dvisc	0.0002563	Pa×s	475.88	Joback Method
dvisc	0.0001358	Pa×s	523.85	Joback Method
dvisc	0.0000800	Pa×s	571.82	Joback Method
dvisc	0.0000512	Pa×s	619.78	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5349633&Units=SI

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