Benzene, 1-(1,1-dimethylethyl)-4-ethoxy-

Other names:	Phenetole, p-tert-butyl-
	p-tert-Butylphenetole
	Ethyl 4-terbutylphenyl ether
	1-(1,1-Dimethylethyl)-4-ethoxy-benzene
Inchi:	InChI=1S/C12H18O/c1-5-13-11-8-6-10(7-9-11)12(2,3)4/h6-9H,5H2,1-4H3
InchiKey:	RMSGBIDKBWPHMJ-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CCOc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	178.27
CAS:	17269-94-2

Physical Properties

Property code	Value	Unit	Source
gf	50.78	kJ/mol	Joback Method
hf	-206.92	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	46.36	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.383		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1728.00		NIST Webbook
tb	524.81	K	Joback Method
tc	736.13	K	Joback Method
tf	288.59	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.40	J/mol×K	524.81	Joback Method
cpg	392.68	J/mol×K	560.03	Joback Method
cpg	408.95	J/mol×K	595.25	Joback Method
cpg	424.27	J/mol×K	630.47	Joback Method

cpg	438.66	J/mol×K	665.69	Joback Method
cpg	452.17	J/mol×K	700.91	Joback Method
cpg	464.83	J/mol×K	736.13	Joback Method
dvisc	0.0025519	Pa×s	288.59	Joback Method
dvisc	0.0012144	Pa×s	327.96	Joback Method
dvisc	0.0006777	Pa×s	367.33	Joback Method
dvisc	0.0004233	Pa×s	406.70	Joback Method
dvisc	0.0002874	Pa×s	446.07	Joback Method
dvisc	0.0002077	Pa×s	485.44	Joback Method
dvisc	0.0001576	Pa×s	524.81	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17269942&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

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