Benzene, 1-ethoxy-2-methyl-

Other names:	Phenetole, o-methyl-
	o-Ethoxytoluene
	Ethyl o-tolyl ether
	1-Ethoxy-2-methylbenzene
	2-Ethoxytoluene
	o-Methylphenetole
Inchi:	InChI=1S/C9H12O/c1-3-10-9-7-5-4-6-8(9)2/h4-7H,3H2,1-2H3
InchiKey:	JWMKUKRBNODZFA-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CCOc1ccccc1C
Mol. weight [g/mol]:	136.19
CAS:	614-71-1

Physical Properties

Property code	Value	Unit	Source
gf	22.68	kJ/mol	Joback Method
hf	-136.25	kJ/mol	Joback Method
hfus	13.91	kJ/mol	Joback Method
hvap	40.98	kJ/mol	Joback Method
ie	8.21	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-2.49		Crippen Method
logp	2.394		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	1054.50		NIST Webbook
rinpol	1054.50		NIST Webbook
tb	458.00 ± 2.00	K	NIST Webbook
tb	457.20	K	NIST Webbook
tc	666.56	K	Joback Method
tf	252.36	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.26	J/mol×K	459.40	Joback Method
cpg	252.44	J/mol×K	493.93	Joback Method
cpg	265.00	J/mol×K	528.45	Joback Method
cpg	276.96	J/mol×K	562.98	Joback Method
cpg	288.33	J/mol×K	597.50	Joback Method
cpg	299.11	J/mol×K	632.03	Joback Method
cpg	309.32	J/mol×K	666.56	Joback Method
dvisc	0.0018481	Pa×s	252.36	Joback Method
dvisc	0.0010126	Pa×s	286.87	Joback Method
dvisc	0.0006314	Pa×s	321.37	Joback Method
dvisc	0.0004314	Pa×s	355.88	Joback Method
dvisc	0.0003153	Pa×s	390.39	Joback Method
dvisc	0.0002425	Pa×s	424.89	Joback Method
dvisc	0.0001940	Pa×s	459.40	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C614711&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ie: Ionization energy
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