

Phenol, 3-ethoxy-

Other names:	Phenol, m-ethoxy- m-Ethoxyphenol Resorcinol monoethyl ether 3-Ethoxyphenol
Inchi:	InChI=1S/C8H10O2/c1-2-10-8-5-3-4-7(9)6-8/h3-6,9H,2H2,1H3
InchiKey:	VBIKLMJHBGFTPV-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	CCOc1cccc(O)c1
Mol. weight [g/mol]:	138.16
CAS:	621-34-1

Physical Properties

Property code	Value	Unit	Source
gf	-130.73	kJ/mol	Joback Method
hf	-281.45	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	51.10	kJ/mol	Joback Method
ie	8.49 ± 0.15	eV	NIST Webbook
log10ws	-1.56		Crippen Method
logp	1.791		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
ripol	2427.00		NIST Webbook
ripol	2427.00		NIST Webbook
tb	519.50 ± 0.50	K	NIST Webbook
tc	735.66	K	Joback Method
tf	340.29	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.89	J/mol×K	512.16	Joback Method
cpg	297.67	J/mol×K	698.41	Joback Method
cpg	288.82	J/mol×K	661.16	Joback Method
cpg	279.38	J/mol×K	623.91	Joback Method
cpg	269.29	J/mol×K	586.66	Joback Method
cpg	258.48	J/mol×K	549.41	Joback Method
cpg	305.97	J/mol×K	735.66	Joback Method
dvisc	0.0000685	Pa×s	512.16	Joback Method
dvisc	0.0001055	Pa×s	483.51	Joback Method
dvisc	0.0001715	Pa×s	454.87	Joback Method
dvisc	0.0002977	Pa×s	426.23	Joback Method
dvisc	0.0005594	Pa×s	397.58	Joback Method
dvisc	0.0011593	Pa×s	368.94	Joback Method
dvisc	0.0027165	Pa×s	340.29	Joback Method

Sources

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=C621341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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