

3-Ethylphenol, methyl ether

Other names:	m-Ethylanisole Benzene, 1-ethyl-3-methoxy- 3-Ethylanisole
Inchi:	InChI=1S/C9H12O/c1-3-8-5-4-6-9(7-8)10-2/h4-7H,3H2,1-2H3
InchiKey:	DWLZULQNIPIABE-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CCc1cccc(OC)c1
Mol. weight [g/mol]:	136.19
CAS:	10568-38-4

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
log10ws	-2.39		Crippen Method
logp	2.258		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1126.20		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1126.20		NIST Webbook
tb	459.40	K	Joback Method
tc	666.56	K	Joback Method
tf	252.36	K	Joback Method
vc	0.450	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.26	J/molxK	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	Paxs	252.36	Joback Method
dvisc	0.0010126	Paxs	286.87	Joback Method
dvisc	0.0006314	Paxs	321.37	Joback Method
dvisc	0.0004314	Paxs	355.88	Joback Method
dvisc	0.0003153	Paxs	390.39	Joback Method
dvisc	0.0002425	Paxs	424.89	Joback Method
dvisc	0.0001940	Paxs	459.40	Joback Method
hvapt	49.30	kJ/mol	388.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	469.70	K	101.00	NIST Webbook

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=C10568384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

h vap:	Enthalpy of vaporization at standard conditions
h vapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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