Phenol, 3-ethyl-5-methyl-

Other names:	1-Hydroxy-3-methyl-5-ethylbenzene
	3-Ethyl-5-methylphenol
	3-Methyl-5-ethylphenol
	5-Ethyl-3-methyphenol
	5-ethyl-m-cresol
	m-Cresol, 5-ethyl-
Inchi:	InChI=1S/C9H12O/c1-3-8-4-7(2)5-9(10)6-8/h4-6,10H,3H2,1-2H3
InchiKey:	XTCHLXABLZQNNN-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CCc1cc(C)cc(O)c1
Mol. weight [g/mol]:	136.19
CAS:	698-71-5

Physical Properties

Property code	Value	Unit	Source
gf	-26.94	kJ/mol	Joback Method
hf	-181.34	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	51.58	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.263		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
ripol	1520.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1520.00		NIST Webbook
tb	517.60	K	Joback Method
tc	740.98	K	Joback Method
tf	341.85	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	322.10	J/mol×K	703.75	Joback Method
cpg	331.15	J/mol×K	740.98	Joback Method
cpg	267.07	J/mol×K	517.60	Joback Method
cpg	279.62	J/mol×K	554.83	Joback Method
cpg	291.33	J/mol×K	592.06	Joback Method
cpg	302.26	J/mol×K	629.29	Joback Method
cpg	312.50	J/mol×K	666.52	Joback Method
dvisc	0.0000711	Pa×s	517.60	Joback Method
dvisc	0.0001085	Pa×s	488.31	Joback Method
dvisc	0.0026759	Pa×s	341.85	Joback Method
dvisc	0.0011514	Pa×s	371.14	Joback Method
dvisc	0.0005605	Pa×s	400.43	Joback Method
dvisc	0.0003010	Pa×s	429.73	Joback Method
dvisc	0.0001750	Pa×s	459.02	Joback Method
hvapt	58.50	kJ/mol	445.50	NIST Webbook
hvapt	55.00	kJ/mol	494.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54470e+01
Coeff. B	-4.61795e+03
Coeff. C	-8.26940e+01
Temperature range (K), min.	387.32
Temperature range (K), max.	538.31

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C698715&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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