

Phenol, 3-ethyl-4-methyl-

Other names:	3-ethyl-p-cresol 3-ethyl-4-methylphenol
Inchi:	InChI=1S/C9H12O/c1-3-8-6-9(10)5-4-7(8)2/h4-6,10H,3H2,1-2H3
InchiKey:	BTRPJOHXPQOVLS-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CCc1cc(O)ccc1C
Mol. weight [g/mol]:	136.19
CAS:	6161-67-7

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
mvol	119.780	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
tb	507.65 ± 3.00	K	NIST Webbook
tb	507.65 ± 3.00	K	NIST Webbook
tb	513.15 ± 4.00	K	NIST Webbook
tc	740.98	K	Joback Method
tf	306.15 ± 3.00	K	NIST Webbook
tf	306.15 ± 3.00	K	NIST Webbook
vc	0.398	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	322.10	J/mol×K	703.75	Joback Method
cpg	331.15	J/mol×K	740.98	Joback Method
dvisc	0.0026759	Paxs	341.85	Joback Method
dvisc	0.0011514	Paxs	371.14	Joback Method
dvisc	0.0005605	Paxs	400.43	Joback Method
dvisc	0.0003010	Paxs	429.73	Joback Method
dvisc	0.0001750	Paxs	459.02	Joback Method
dvisc	0.0001085	Paxs	488.31	Joback Method
dvisc	0.0000711	Paxs	517.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6161677&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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