

Phenol, 2-ethyl-5-methyl-

Other names:	m-Cresol, 6-ethyl- 2-Ethyl-5-methylphenol Ethyl-m-cresol 6-Ethyl-m-cresol 5-Ethyl-2-methylphenol
Inchi:	InChI=1S/C9H12O/c1-3-8-5-4-7(2)6-9(8)10/h4-6,10H,3H2,1-2H3
InchiKey:	LTRVUFFOMIUCPJ-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CCc1ccc(C)cc1O
Mol. weight [g/mol]:	136.19
CAS:	1687-61-2

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
tb	497.35 ± 3.00	K	NIST Webbook
tb	498.35 ± 3.00	K	NIST Webbook
tb	497.35 ± 3.00	K	NIST Webbook
tb	497.35 ± 3.00	K	NIST Webbook
tc	740.98	K	Joback Method
tf	316.55 ± 2.00	K	NIST Webbook
tf	315.65 ± 2.00	K	NIST Webbook
tf	316.55 ± 2.00	K	NIST Webbook
vc	0.398	m3/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	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
dvisc	0.0001085	Pa×s	488.31	Joback Method
dvisc	0.0000711	Pa×s	517.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1687612&Units=SI

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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