Phenol, 2-ethyl-6-methyl-

Other names: o-Cresol, 6-ethyl-
2-Ethyl-6-methylphenol
6-Ethyl-o-cresol
Inchi: InChI=1S/C9H12O/c1-3-8-6-4-5-7(2)9(8)10/h4-6,10H,3H2,1-2H3
InchiKey: CIRRFAQIWQFQSS-UHFFFAOYSA-N
Formula: C9H12O
SMILES: CCc1cccc(C)c1O
Mol. weight [g/mol]: 136.19
CAS: 1687-64-5

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
rinpol	1236.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1236.00		NIST Webbook
ripol	2170.00		NIST Webbook
tb	486.15 ± 3.00	K	NIST Webbook
tb	486.15 ± 3.00	K	NIST Webbook
tb	486.15 ± 3.00	K	NIST Webbook
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	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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1687645&Units=SI
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
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

Latest version available from:
https://www.chemeo.com/cid/11-994-6/Phenol-2-ethyl-6-methyl.pdf
Generated by Cheméo on 2025-12-05 14:46:10.487943637 +0000 UTC m=+4694168.017984303.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.