Phenol, 2-ethyl-4,5-dimethyl-

Other names:	3,4-Xylenol, 6-ethyl-
	6-Ethyl-3,4-dimethylphenol
	1-Hydroxy-3,4-dimethyl-6-ethylbenzene
	4,5-Dimethyl-2-ethylphenol
	2-ethyl-4,5-dimethylphenol
Inchi:	InChI=1S/C10H14O/c1-4-9-5-7(2)8(3)6-10(9)11/h5-6,11H,4H2,1-3H3
InchiKey:	ZUDAICPAUJSPHK-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CCc1cc(C)c(C)cc1O
Mol. weight [g/mol]:	150.22
CAS:	2219-78-5

Physical Properties

Property code	Value	Unit	Source
gf	-28.15	kJ/mol	Joback Method
hf	-213.45	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	54.47	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.571		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	1305.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1313.00		NIST Webbook
tb	523.15 ± 5.00	K	NIST Webbook
tc	766.07	K	Joback Method
tf	324.65 ± 2.00	K	NIST Webbook
tf	324.65 ± 2.00	K	NIST Webbook
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.96	J/mol×K	545.46	Joback Method
cpg	369.35	J/mol×K	729.30	Joback Method
cpg	359.01	J/mol×K	692.53	Joback Method
cpg	348.06	J/mol×K	655.76	Joback Method
cpg	336.45	J/mol×K	619.00	Joback Method
cpg	324.10	J/mol×K	582.23	Joback Method
cpg	379.14	J/mol×K	766.07	Joback Method
dvisc	0.0000533	Pa×s	545.46	Joback Method
dvisc	0.0000790	Pa×s	515.49	Joback Method
dvisc	0.0001229	Pa×s	485.52	Joback Method
dvisc	0.0002028	Pa×s	455.55	Joback Method
dvisc	0.0003591	Pa×s	425.58	Joback Method
dvisc	0.0006933	Pa×s	395.61	Joback Method
dvisc	0.0014909	Pa×s	365.64	Joback Method

Sources

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=C2219785&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume