

Phenol, 4-ethyl-2,6-dimethoxy

Other names:	4-Ethylsyringol Syringol, 4-ethyl 4-Ethyl-2,6-dimethoxyphenol (4-ethylsyringol) 2,6-Dimethoxy-4-ethyl-phenol
Inchi:	InChI=1S/C10H14O3/c1-4-7-5-8(12-2)10(11)9(6-7)13-3/h5-6,11H,4H2,1-3H3
InchiKey:	PJWDIHUFLXQRFF-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CCc1cc(OC)c(O)c(OC)c1
Mol. weight [g/mol]:	182.22

Physical Properties

Property code	Value	Unit	Source
gf	-238.15	kJ/mol	Joback Method
hf	-477.89	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	59.29	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.972		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1557.00		NIST Webbook
ripol	2404.00		NIST Webbook
tb	590.30	K	Joback Method
tc	805.71	K	Joback Method
tf	410.10	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.08	J/molxK	590.30	Joback Method
cpg	415.37	J/molxK	769.81	Joback Method
cpg	405.08	J/molxK	733.90	Joback Method

cpg	394.24	J/molxK	698.00	Joback Method
cpg	382.81	J/molxK	662.10	Joback Method
cpg	370.77	J/molxK	626.20	Joback Method
cpg	425.12	J/molxK	805.71	Joback Method
dvisc	0.0000270	Paxs	590.30	Joback Method
dvisc	0.0000386	Paxs	560.27	Joback Method
dvisc	0.0000575	Paxs	530.23	Joback Method
dvisc	0.0000898	Paxs	500.20	Joback Method
dvisc	0.0001485	Paxs	470.17	Joback Method
dvisc	0.0002630	Paxs	440.13	Joback Method
dvisc	0.0005067	Paxs	410.10	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=R14541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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