4-Propylsyringol

Other names:	Phenol, 4-propyl-2,6-dimethoxy
	Phenol, 2,6-dimethoxy-4-propyl
	4-Propyl-2,6-dimethoxyphenol (4-propylsyringol)
Inchi:	InChI=1S/C11H16O3/c1-4-5-8-6-9(13-2)11(12)10(7-8)14-3/h6-7,12H,4-5H2,1-3H3
InchiKey:	YHEWWEXPVKCVFY-UHFFFAOYSA-N
Formula:	C11H16O3
SMILES:	CCCc1cc(OC)c(O)c(OC)c1
Mol. weight [g/mol]:	196.24

Physical Properties

Property code	Value	Unit	Source
gf	-229.73	kJ/mol	Joback Method
hf	-498.53	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	61.51	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.362		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1568.00		NIST Webbook
tb	613.18	K	Joback Method
tc	824.99	K	Joback Method
tf	421.37	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.88	J/mol×K	613.18	Joback Method
cpg	419.38	J/mol×K	648.48	Joback Method
cpg	432.21	J/mol×K	683.78	Joback Method
cpg	444.38	J/mol×K	719.09	Joback Method
cpg	455.93	J/mol×K	754.39	Joback Method
cpg	466.88	J/mol×K	789.69	Joback Method
cpg	477.28	J/mol×K	824.99	Joback Method
dvisc	0.0004325	Pa×s	421.37	Joback Method
dvisc	0.0002202	Pa×s	453.34	Joback Method
dvisc	0.0001225	Pa×s	485.31	Joback Method
dvisc	0.0000733	Pa×s	517.28	Joback Method
dvisc	0.0000466	Pa×s	549.24	Joback Method
dvisc	0.0000311	Pa×s	581.21	Joback Method
dvisc	0.0000216	Pa×s	613.18	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=R14555&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