Phenol, 3-propyl-

Other names:	1-Hydroxy-3-n-propylbenzene
	3-Propylphenol
	3-n-Propylphenol
	Phenol, m-propyl-
	m-Propylphenol
Inchi:	InChI=1S/C9H12O/c1-2-4-8-5-3-6-9(10)7-8/h3,5-7,10H,2,4H2,1H3
InchiKey:	MPWGZBWDLMDIHO-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CCCc1cccc(O)c1
Mol. weight [g/mol]:	136.19
CAS:	621-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-17.31	kJ/mol	Joback Method
hf	-169.87	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	50.92	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.345		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1236.00		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2246.00		NIST Webbook
ripol	2250.00		NIST Webbook
tb	501.15 ± 3.00	K	NIST Webbook
tb	501.15 ± 3.00	K	NIST Webbook
tb	504.15 ± 3.00	K	NIST Webbook
tb	501.15 ± 3.00	K	NIST Webbook
tc	734.79	K	Joback Method
tf	299.15 ± 2.00	K	NIST Webbook
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.43	J/mol×K	623.70	Joback Method
cpg	332.77	J/mol×K	734.79	Joback Method
cpg	323.62	J/mol×K	697.76	Joback Method
cpg	313.87	J/mol×K	660.73	Joback Method
cpg	267.25	J/mol×K	512.62	Joback Method
cpg	280.20	J/mol×K	549.65	Joback Method
cpg	292.23	J/mol×K	586.68	Joback Method
dvisc	0.0000766	Pa×s	512.62	Joback Method
dvisc	0.0003692	Pa×s	420.98	Joback Method
dvisc	0.0002036	Pa×s	451.52	Joback Method
dvisc	0.0001211	Pa×s	482.07	Joback Method
dvisc	0.0042723	Pa×s	329.33	Joback Method
dvisc	0.0016445	Pa×s	359.88	Joback Method
dvisc	0.0007350	Pa×s	390.43	Joback Method
hvapt	53.00	kJ/mol	449.00	NIST Webbook
hvapt	57.20	kJ/mol	449.00	NIST Webbook
hvapt	59.90	kJ/mol	449.00	NIST Webbook
hvapt	60.20	kJ/mol	473.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55321e+01
Coeff. B	-4.58817e+03
Coeff. C	-8.07480e+01
Temperature range (K), min.	381.72
Temperature range (K), max.	529.66

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=C621272&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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