

2-propylresorcinol

Inchi:	InChI=1S/C9H12O2/c1-2-4-7-8(10)5-3-6-9(7)11/h3,5-6,10-11H,2,4H2,1H3
InchiKey:	XDCMHOFEBFTMNL-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CCc1c(O)cccc1O
Mol. weight [g/mol]:	152.19

Physical Properties

Property code	Value	Unit	Source
gf	-171.93	kJ/mol	Joback Method
hf	-347.18	kJ/mol	Joback Method
hfus	24.67	kJ/mol	Joback Method
hvap	63.93	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	2.050		Crippen Method
mvol	125.650	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
tb	593.24	K	Joback Method
tc	826.79	K	Joback Method
tf	377.90	K	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.64	J/molxK	593.24	Joback Method
cpg	325.87	J/molxK	632.17	Joback Method
cpg	336.27	J/molxK	671.09	Joback Method
cpg	345.97	J/molxK	710.02	Joback Method
cpg	355.11	J/molxK	748.94	Joback Method
cpg	363.83	J/molxK	787.87	Joback Method

cpg	372.27	J/molxK	826.79	Joback Method
dvisc	0.0002757	Paxs	441.05	Joback Method
dvisc	0.0001281	Paxs	466.42	Joback Method
dvisc	0.0000644	Paxs	491.78	Joback Method
dvisc	0.0000346	Paxs	517.14	Joback Method
dvisc	0.0000197	Paxs	542.51	Joback Method
dvisc	0.0000118	Paxs	567.88	Joback Method
dvisc	0.0000074	Paxs	593.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	470.60	K	9.92	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
tbp	491.40	K	19.83	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
tbp	504.70	K	29.79	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry

tbp	523.40	K	49.69	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
tbp	536.40	K	69.61	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
tbp	551.10	K	98.91	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
tbp	582.80	K	198.31	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
tbp	605.40	K	299.37	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry

tbp	618.90	K	400.46	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
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Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry:	https://www.doi.org/10.1016/j.jct.2019.03.008

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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