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: CCCc1c(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
mcvol	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/mol×K	593.24	Joback Method
cpg	325.87	J/mol×K	632.17	Joback Method
cpg	336.27	J/mol×K	671.09	Joback Method
cpg	345.97	J/mol×K	710.02	Joback Method
cpg	355.11	J/mol×K	748.94	Joback Method
cpg	363.83	J/mol×K	787.87	Joback Method

cpg	372.27	J/mol×K	826.79	Joback Method
dvisc	0.0002757	Pa×s	441.05	Joback Method
dvisc	0.0001281	Pa×s	466.42	Joback Method
dvisc	0.0000644	Pa×s	491.78	Joback Method
dvisc	0.0000346	Pa×s	517.14	Joback Method
dvisc	0.0000197	Pa×s	542.51	Joback Method
dvisc	0.0000118	Pa×s	567.88	Joback Method
dvisc	0.0000074	Pa×s	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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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