2-Allylphenol

Other names: Phenol, o-allyl-
Phenol, 2-(propenyl)-
o-Allylphenol
2-(2-Propenyl)-phenol
Phenol, 2-(2-propenyl)-
Inchi: InChI=1S/C9H10O/c1-2-5-8-6-3-4-7-9(8)10/h2-4,6-7,10H,1,5H2
InchiKey: QIRNGVVZBINFMX-UHFFFAOYSA-N
Formula: C9H10O
SMILES: C=CCc1ccccc1O
Mol. weight [g/mol]: 134.18
CAS: 1745-81-9

Physical Properties

Property code	Value	Unit	Source
gf	70.53	kJ/mol	Joback Method
hf	-44.44	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	50.25	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.121		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	192.80		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	192.80		NIST Webbook
ripol	2039.00		NIST Webbook
ripol	2132.00		NIST Webbook
tb	493.20	K	NIST Webbook
tb	493.00 ± 5.00	K	NIST Webbook
tc	736.53	K	Joback Method
tf	327.57	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.21	J/mol×K	509.30	Joback Method
cpg	261.41	J/mol×K	547.17	Joback Method
cpg	272.66	J/mol×K	585.04	Joback Method
cpg	283.06	J/mol×K	622.91	Joback Method
cpg	292.68	J/mol×K	660.78	Joback Method
cpg	301.63	J/mol×K	698.65	Joback Method
cpg	309.98	J/mol×K	736.53	Joback Method
dvisc	0.0042028	Pa×s	327.57	Joback Method
dvisc	0.0016414	Pa×s	357.86	Joback Method
dvisc	0.0007423	Pa×s	388.15	Joback Method
dvisc	0.0003766	Pa×s	418.44	Joback Method
dvisc	0.0002094	Pa×s	448.72	Joback Method
dvisc	0.0001254	Pa×s	479.01	Joback Method
dvisc	0.0000798	Pa×s	509.30	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1745819&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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