

Phenol, 2-ethenyl-

Inchi:	InChI=1S/C8H8O/c1-2-7-5-3-4-6-8(7)9/h2-6,9H,1H2
InchiKey:	JESXATFQYMPTNL-UHFFFAOYSA-N
Formula:	C8H8O
SMILES:	C=Cc1ccccc1O
Mol. weight [g/mol]:	120.15
CAS:	695-84-1

Physical Properties

Property code	Value	Unit	Source
gf	62.11	kJ/mol	Joback Method
hf	-23.80	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	48.02	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	2.035		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
rinpol	1141.00		NIST Webbook
rinpol	1141.00		NIST Webbook
ripol	2203.00		NIST Webbook
tb	486.42	K	Joback Method
tc	717.70	K	Joback Method
tf	302.40 ± 1.00	K	NIST Webbook
tf	302.40 ± 0.60	K	NIST Webbook
vc	0.323	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.55	J/mol×K	486.42	Joback Method
cpg	218.69	J/mol×K	524.97	Joback Method
cpg	228.90	J/mol×K	563.51	Joback Method
cpg	238.27	J/mol×K	602.06	Joback Method
cpg	246.89	J/mol×K	640.60	Joback Method

cpg	254.86	J/mol×K	679.15	Joback Method
cpg	262.25	J/mol×K	717.70	Joback Method
dvisc	0.0050655	Paxs	316.30	Joback Method
dvisc	0.0020148	Paxs	344.65	Joback Method
dvisc	0.0009219	Paxs	373.01	Joback Method
dvisc	0.0004711	Paxs	401.36	Joback Method
dvisc	0.0002631	Paxs	429.71	Joback Method
dvisc	0.0001579	Paxs	458.07	Joback Method
dvisc	0.0001006	Paxs	486.42	Joback Method

Sources

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=C695841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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