

Coahuilensol (Phenol, 2-ethenyl-3-methyl)

Inchi:	InChI=1S/C9H10O/c1-3-8-7(2)5-4-6-9(8)10/h3-6,10H,1H2,2H3
InchiKey:	MCBGBITUMUAJMT-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	C=Cc1c(C)cccc1O
Mol. weight [g/mol]:	134.18

Physical Properties

Property code	Value	Unit	Source
gf	60.90	kJ/mol	Joback Method
hf	-55.91	kJ/mol	Joback Method
hfus	17.22	kJ/mol	Joback Method
hvap	50.91	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.344		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	1177.00		NIST Webbook
tb	514.28	K	Joback Method
tc	742.74	K	Joback Method
tf	340.09	K	Joback Method
vc	0.379	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.93	J/molxK	514.28	Joback Method
cpg	260.71	J/molxK	552.36	Joback Method
cpg	271.62	J/molxK	590.43	Joback Method
cpg	281.74	J/molxK	628.51	Joback Method
cpg	291.16	J/molxK	666.59	Joback Method
cpg	299.95	J/molxK	704.66	Joback Method
cpg	308.20	J/molxK	742.74	Joback Method
dvisc	0.0026381	Paxs	340.09	Joback Method
dvisc	0.0011507	Paxs	369.12	Joback Method

dvisc	0.0005665	Paxs	398.15	Joback Method
dvisc	0.0003071	Paxs	427.19	Joback Method
dvisc	0.0001799	Paxs	456.22	Joback Method
dvisc	0.0001124	Paxs	485.25	Joback Method
dvisc	0.0000741	Paxs	514.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R568864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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