Ethchlorvynol

Other names:	1-Penten-4-yn-3-ol, 1-chloro-3-ethyl-
	Alvinol
	Ethchlorovynol
	Ethchlorvinol
	Ethochlorvynol
	Ethyl «beta»-chlorovinyl ethynyl carbinol
	Normosan
	Normoson
	Nostel
	Placidyl
	Serensil
	«beta»-Chlorovinyl ethyl ethynyl carbinol
	A 71
	Aethyl-chlorvynol
	Arvynol
	Etchlorvinolo
	Ethchlorvinyl
	Ethychlorvynol
	Normonson
	Placidil
	Roeridorm
	Serenil
	1-Chloro-3-ethyl-1-penten-4-yn-3-ol
	3-(«beta»-chlorovinyl)-1-pentyn-3-ol
	Ethclorvynol
	Serensiloline
	Nromoson
	Serenesil
	NSC 30372
	(1E)-1-Chloro-3-ethyl-1-penten-4-yn-3-ol
Inchi:	InChI=1S/C7H9ClO/c1-3-7(9,4-2)5-6-8/h1,5-6,9H,4H2,2H3/b6-5+
InchiKey:	ZEHYJZXQEQOSON-AATRIKPKSA-N
Formula:	C7H9ClO
SMILES:	C#CC(O)(C=CCl)CC
Mol. weight [g/mol]:	144.60
CAS:	113-18-8

Physical Properties

Property code	Value	Unit	Source
gf	165.44	kJ/mol	Joback Method
hf	44.59	kJ/mol	Joback Method
hfus	17.93	kJ/mol	Joback Method
hvap	50.76	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.513		Crippen Method
mcvol	114.700	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
rinpol	1023.00		NIST Webbook
rinpol	1005.60		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1005.60		NIST Webbook
rinpol	1030.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1445.00		NIST Webbook
tb	480.22	K	Joback Method
tc	676.92	K	Joback Method
tf	303.70	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.79	J/mol×K	480.22	Joback Method
cpg	237.84	J/mol×K	513.00	Joback Method
cpg	246.22	J/mol×K	545.79	Joback Method
cpg	253.99	J/mol×K	578.57	Joback Method
cpg	261.19	J/mol×K	611.35	Joback Method
cpg	267.88	J/mol×K	644.14	Joback Method
cpg	274.10	J/mol×K	676.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C113188&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
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