Prenol

Other names:	2-Buten-1-ol, 3-methyl-
	2-Butenol, 3-methyl
	3,3-Dimethylallyl alcohol
	3-Methyl-2-buten-1-ol
	3-Methyl-2-butene-1-ol
	3-Methyl-2-butenol
	3-Methyl-2-butenyl alcohol
	3-Methylbut-2-en-1-ol
	3-Methylcrotyl alcohol
	Dimethylallyl alcohol
	Methyl-3-but-2-en-1-ol
	NSC 158709
	Prenyl alcohol
	«gamma»,«gamma»-Dimethylallyl alcohol
	Â«gammaÂ»,Â«gammaÂ»-Dimethylallyl alcohol
Inchi:	InChI=1S/C5H10O/c1-5(2)3-4-6/h3,6H,4H2,1-2H3
InchiKey:	ASUAYTHWZCLXAN-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CC(C)=CCO
Mol. weight [g/mol]:	86.13
CAS:	556-82-1

Physical Properties

Property code	Value	Unit	Source
gf	-73.93	kJ/mol	Joback Method
hf	-191.33	kJ/mol	Joback Method
hfus	11.69	kJ/mol	Joback Method
hvap	43.44	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	0.945		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
rinpol	770.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	785.60		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	779.00		NIST Webbook

rinpol	778.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	784.10	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	767.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	762.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	770.00	NIST Webbook
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rinpol	765.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	765.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	786.60	NIST Webbook
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rinpol	751.00	NIST Webbook
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rinpol	752.00	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	732.00	NIST Webbook

rinpol	789.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	770.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	763.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	778.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1327.00	NIST Webbook
ripol	1320.00	NIST Webbook
ripol	1277.00	NIST Webbook
ripol	1323.00	NIST Webbook
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ripol	1316.00	NIST Webbook
ripol	1313.00	NIST Webbook
ripol	1281.00	NIST Webbook
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ripol	1327.00	NIST Webbook
ripol	1317.00	NIST Webbook

ripol	1328.00		NIST Webbook
ripol	1311.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1346.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1328.00		NIST Webbook
tb	413.20	K	NIST Webbook
tc	582.88	K	Joback Method
tf	187.89	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.28	J/mol×K	410.02	Joback Method
cpg	162.38	J/mol×K	438.83	Joback Method
cpg	170.11	J/mol×K	467.64	Joback Method
cpg	177.48	J/mol×K	496.45	Joback Method
cpg	184.52	J/mol×K	525.26	Joback Method
cpg	191.23	J/mol×K	554.07	Joback Method
cpg	197.63	J/mol×K	582.88	Joback Method
hvapt	48.70	kJ/mol	360.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59002e+01
Coeff. B	-4.02983e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	314.12
Temperature range (K), max.	436.58

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C556821&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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