

3-Penten-2-ol

Other names:	3-Penten-2-ol,cis+trans 3-Pentene-2-ol Methyl propenyl carbinol Pent-3-en-2-ol «alpha», «gamma»-Dimethylallyl alcohol Â«alphaÂ», Â«gammaÂ»-Dimethylallyl alcohol
Inchi:	InChI=1S/C5H10O/c1-3-4-5(2)6/h3-6H,1-2H3
InchiKey:	GJYMQFMQRRNLCY-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CC=CC(C)O
Mol. weight [g/mol]:	86.13
CAS:	1569-50-2

Physical Properties

Property code	Value	Unit	Source
gf	-67.82	kJ/mol	Joback Method
hf	-186.82	kJ/mol	Joback Method
hfus	9.47	kJ/mol	Joback Method
hvap	42.97	kJ/mol	Joback Method
ie	9.56	eV	NIST Webbook
log10ws	-1.14		Crippen Method
logp	0.943		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
ripol	774.00		NIST Webbook
ripol	774.00		NIST Webbook
ripol	774.00		NIST Webbook
ripol	1172.00		NIST Webbook
ripol	1182.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1174.00		NIST Webbook
ripol	1170.00		NIST Webbook

ripol	1177.00		NIST Webbook
ripol	1174.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1170.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1170.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1182.00		NIST Webbook
tb	395.80 ± 4.00	K	NIST Webbook
tb	393.20	K	NIST Webbook
tc	583.15	K	Joback Method
tf	186.85	K	Joback Method
vc	0.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.35	J/molxK	409.70	Joback Method
cpg	162.59	J/molxK	438.61	Joback Method
cpg	170.46	J/molxK	467.52	Joback Method
cpg	177.96	J/molxK	496.43	Joback Method
cpg	185.11	J/molxK	525.33	Joback Method
cpg	191.93	J/molxK	554.24	Joback Method
cpg	198.43	J/molxK	583.15	Joback Method
dvisc	0.3400407	Paxs	186.85	Joback Method
dvisc	0.0364983	Paxs	223.99	Joback Method
dvisc	0.0073915	Paxs	261.13	Joback Method
dvisc	0.0022280	Paxs	298.27	Joback Method
dvisc	0.0008759	Paxs	335.42	Joback Method
dvisc	0.0004148	Paxs	372.56	Joback Method
dvisc	0.0002249	Paxs	409.70	Joback Method

Correlations

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.59654e+01
Coeff. B	-3.88927e+03
Coeff. C	-5.04460e+01
Temperature range (K), min.	298.52
Temperature range (K), max.	415.50

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1569502&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/ci9903071
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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