

1-Penten-3-ol, 2-methyl-

Other names:	2-Methyl-1-penten-3-ol Propanol, 1-ethyl-2-methylene-
Inchi:	InChI=1S/C6H12O/c1-4-6(7)5(2)3/h6-7H,2,4H2,1,3H3
InchiKey:	DHNPVHJGKASNBQ-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	C=C(C)C(O)CC
Mol. weight [g/mol]:	100.16
CAS:	2088-07-5

Physical Properties

Property code	Value	Unit	Source
gf	-60.33	kJ/mol	Joback Method
hf	-209.04	kJ/mol	Joback Method
hfus	9.27	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.333		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
rinpol	776.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	776.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1382.00		NIST Webbook
tb	424.98	K	Joback Method
tc	595.89	K	Joback Method
tf	187.48	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.18	J/molxK	424.98	Joback Method
cpg	201.51	J/molxK	453.46	Joback Method

cpg	210.45	J/mol×K	481.95	Joback Method
cpg	219.01	J/mol×K	510.43	Joback Method
cpg	227.21	J/mol×K	538.92	Joback Method
cpg	235.05	J/mol×K	567.40	Joback Method
cpg	242.55	J/mol×K	595.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2088075&Units=SI

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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