

5-Hexen-2-ol, 5-methyl-

Other names:	5-Methyl-5-hexen-2-ol
Inchi:	InChI=1S/C7H14O/c1-6(2)4-5-7(3)8/h7-8H,1,4-5H2,2-3H3
InchiKey:	RIEDLCPIEKXTTL-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	C=C(C)CCC(C)O
Mol. weight [g/mol]:	114.19
CAS:	50551-88-7

Physical Properties

Property code	Value	Unit	Source
gf	-51.91	kJ/mol	Joback Method
hf	-229.68	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	46.88	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	447.86	K	Joback Method
tc	617.74	K	Joback Method
tf	198.75	K	Joback Method
vc	0.422	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.50	J/molxK	447.86	Joback Method
cpg	241.95	J/molxK	476.17	Joback Method
cpg	251.95	J/molxK	504.49	Joback Method
cpg	261.54	J/molxK	532.80	Joback Method
cpg	270.72	J/molxK	561.11	Joback Method
cpg	279.50	J/molxK	589.43	Joback Method
cpg	287.90	J/molxK	617.74	Joback Method

Sources

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=C50551887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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