

5-Hexen-2-ol

Other names:	Methyl(2-vinylethyl)carbinol 1-Hexen-5-ol 5-Hydroxy-1-hexene
Inchi:	InChI=1S/C6H12O/c1-3-4-5-6(2)7/h3,6-7H,1,4-5H2,2H3
InchiKey:	LNPXWKVAFKIBX-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	C=CCCC(C)O
Mol. weight [g/mol]:	100.16
CAS:	626-94-8

Physical Properties

Property code	Value	Unit	Source
gf	-51.78	kJ/mol	Joback Method
hf	-199.25	kJ/mol	Joback Method
hfus	10.58	kJ/mol	Joback Method
hvap	44.57	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.333		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
rinpola	732.00		NIST Webbook
rinpola	732.00		NIST Webbook
tb	425.10	K	Joback Method
tc	592.88	K	Joback Method
tf	201.44	K	Joback Method
vc	0.365	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.23	J/molxK	425.10	Joback Method
cpg	201.41	J/molxK	453.06	Joback Method
cpg	210.23	J/molxK	481.03	Joback Method
cpg	218.68	J/molxK	508.99	Joback Method

cpg	226.77	J/molxK	536.95	Joback Method
cpg	234.52	J/molxK	564.91	Joback Method
cpg	241.94	J/molxK	592.88	Joback Method
dvisc	0.1985438	Paxs	201.44	Joback Method
dvisc	0.0271287	Paxs	238.72	Joback Method
dvisc	0.0063461	Paxs	275.99	Joback Method
dvisc	0.0020977	Paxs	313.27	Joback Method
dvisc	0.0008774	Paxs	350.55	Joback Method
dvisc	0.0004340	Paxs	387.82	Joback Method
dvisc	0.0002428	Paxs	425.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626948&Units=SI
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

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

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