

(Z)-3-Hexen-2-ol

Inchi:	InChI=1S/C6H12O/c1-3-4-5-6(2)7/h4-7H,3H2,1-2H3/b5-4-
InchiKey:	SMOVOSVEEFIBSP-PLNGDYQASA-N
Formula:	C6H12O
SMILES:	CCC=CC(C)O
Mol. weight [g/mol]:	100.16

Physical Properties

Property code	Value	Unit	Source
gf	-59.40	kJ/mol	Joback Method
hf	-207.46	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	45.20	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.333		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	853.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	853.00		NIST Webbook
tb	432.58	K	Joback Method
tc	605.02	K	Joback Method
tf	198.12	K	Joback Method
vc	0.364	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.87	J/molxK	432.58	Joback Method
cpg	234.96	J/molxK	576.28	Joback Method
cpg	227.13	J/molxK	547.54	Joback Method
cpg	218.92	J/molxK	518.80	Joback Method
cpg	210.32	J/molxK	490.06	Joback Method
cpg	201.31	J/molxK	461.32	Joback Method
cpg	242.44	J/molxK	605.02	Joback Method

dvisc	0.0001926	Paxs	432.58	Joback Method
dvisc	0.0003506	Paxs	393.50	Joback Method
dvisc	0.0007282	Paxs	354.43	Joback Method
dvisc	0.0018131	Paxs	315.35	Joback Method
dvisc	0.0058431	Paxs	276.27	Joback Method
dvisc	0.0276896	Paxs	237.20	Joback Method
dvisc	0.2423961	Paxs	198.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R642185&Units=SI
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
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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