

3,5-Hexadien-2-ol, 2-methyl-

Inchi:	InChI=1S/C7H12O/c1-4-5-6-7(2,3)8/h4-6,8H,1H2,2-3H3/b6-5+
InchiKey:	ZWRDKAOHFUSUWQC-AATRIKPKSA-N
Formula:	C7H12O
SMILES:	C=CC=CC(C)(C)O
Mol. weight [g/mol]:	112.17
CAS:	926-38-5

Physical Properties

Property code	Value	Unit	Source
gf	42.14	kJ/mol	Joback Method
hf	-106.14	kJ/mol	Joback Method
hfus	9.48	kJ/mol	Joback Method
hvap	45.85	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.499		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
tb	449.35	K	Joback Method
tc	630.97	K	Joback Method
tf	225.05	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.90	J/molxK	449.35	Joback Method
cpg	228.54	J/molxK	479.62	Joback Method
cpg	238.54	J/molxK	509.89	Joback Method
cpg	247.93	J/molxK	540.16	Joback Method
cpg	256.75	J/molxK	570.43	Joback Method
cpg	265.03	J/molxK	600.70	Joback Method
cpg	272.82	J/molxK	630.97	Joback Method
dvisc	0.0990503	Paxs	225.05	Joback Method
dvisc	0.0164039	Paxs	262.43	Joback Method

dvisc	0.0042538	Paxs	299.82	Joback Method
dvisc	0.0014879	Paxs	337.20	Joback Method
dvisc	0.0006419	Paxs	374.58	Joback Method
dvisc	0.0003225	Paxs	411.97	Joback Method
dvisc	0.0001817	Paxs	449.35	Joback Method

Sources

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=C926385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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