

2-Methyl-1,5-heptadien-4-ol

Inchi:	InChI=1S/C8H14O/c1-4-5-8(9)6-7(2)3/h4-5,8-9H,2,6H2,1,3H3/b5-4+
InchiKey:	MDTLRZIDFDKYHS-SNAWJCMRSA-N
Formula:	C8H14O
SMILES:	C=C(C)CC(O)C=CC
Mol. weight [g/mol]:	126.20
CAS:	926-98-7

Physical Properties

Property code	Value	Unit	Source
gf	36.73	kJ/mol	Joback Method
hf	-133.10	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	49.06	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.890		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	474.90	K	Joback Method
tc	651.32	K	Joback Method
tf	204.94	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.19	J/molxK	474.90	Joback Method
cpg	267.25	J/molxK	504.30	Joback Method
cpg	277.77	J/molxK	533.71	Joback Method
cpg	287.78	J/molxK	563.11	Joback Method
cpg	297.30	J/molxK	592.52	Joback Method
cpg	306.35	J/molxK	621.92	Joback Method
cpg	314.95	J/molxK	651.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C926987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
mccvol:	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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