

6-Hepten-3-ol, 4-methyl-

Other names:	4-Methyl-6-hepten-3-ol
Inchi:	InChI=1S/C8H16O/c1-4-6-7(3)8(9)5-2/h4,7-9H,1,5-6H2,2-3H3
InchiKey:	QMMJAABEFZXPBD-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	C=CCC(C)C(O)CC
Mol. weight [g/mol]:	128.21
CAS:	53907-71-4

Physical Properties

Property code	Value	Unit	Source
gf	-37.38	kJ/mol	Joback Method
hf	-245.81	kJ/mol	Joback Method
hfus	12.24	kJ/mol	Joback Method
hvap	48.64	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.969		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	986.00		NIST Webbook
rinpol	986.00		NIST Webbook
tb	470.42	K	Joback Method
tc	639.72	K	Joback Method
tf	208.98	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.23	J/mol×K	470.42	Joback Method
cpg	326.46	J/mol×K	611.50	Joback Method
cpg	316.73	J/mol×K	583.29	Joback Method
cpg	306.56	J/mol×K	555.07	Joback Method
cpg	295.93	J/mol×K	526.85	Joback Method
cpg	284.82	J/mol×K	498.64	Joback Method

cpg	335.76	J/mol×K	639.72	Joback Method
dvisc	0.0001650	Paxs	470.42	Joback Method
dvisc	0.0003026	Paxs	426.85	Joback Method
dvisc	0.0006368	Paxs	383.27	Joback Method
dvisc	0.0016221	Paxs	339.70	Joback Method
dvisc	0.0054407	Paxs	296.13	Joback Method
dvisc	0.0277058	Paxs	252.55	Joback Method
dvisc	0.2781497	Paxs	208.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53907714&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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