3-Methyl-5-hexen-3-ol

Other names: Methylaethylallylcarbinol
Methylethylallylcarbinol
Inchi: InChI=1S/C7H14O/c1-4-6-7(3,8)5-2/h4,8H,1,5-6H2,2-3H3
InchiKey: GBARKLJMQRUBKV-UHFFFAOYSA-N
Formula: C7H14O
SMILES: C=CCC(C)(O)CC
Mol. weight [g/mol]: 114.19
CAS: 1569-44-4

Physical Properties

Property code	Value	Unit	Source
hf	-273.86	kJ/mol	Cheméo Relay (1.0)
hfus	9.28	kJ/mol	Joback Method
hvap	52.50	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-0.56		Cheméo Relay (1.0)
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	408.62	K	Cheméo Relay (1.0)
tc	590.82	K	Cheméo Relay (1.0)
tf	210.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.09	J/mol×K	445.19	Joback Method
cpg	245.12	J/mol×K	474.08	Joback Method
cpg	255.60	J/mol×K	502.96	Joback Method
cpg	265.53	J/mol×K	531.85	Joback Method
cpg	274.94	J/mol×K	560.74	Joback Method
cpg	283.87	J/mol×K	589.63	Joback Method
cpg	292.33	J/mol×K	618.51	Joback Method
dvisc	0.0922078	Pa×s	230.13	Joback Method

dvisc	0.0172289	Pa×s	265.97	Joback Method
dvisc	0.0047949	Pa×s	301.82	Joback Method
dvisc	0.0017508	Pa×s	337.66	Joback Method
dvisc	0.0007757	Pa×s	373.50	Joback Method
dvisc	0.0003963	Pa×s	409.35	Joback Method
dvisc	0.0002256	Pa×s	445.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40892e+01
Coeff. B	-3.69927e+03
Coeff. C	-6.12880e+01
Temperature range (K), min.	299.15
Temperature range (K), max.	482.73

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1569444&Units=SI

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point