

5-Methyl-1-hexyn-3-ol

Inchi:	InChI=1S/C7H12O/c1-4-7(8)5-6(2)3/h1,6-8H,5H2,2-3H3
InchiKey:	NTNUBJHPRAMQPC-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	C#CC(O)CC(C)C
Mol. weight [g/mol]:	112.17
CAS:	61996-79-0

Physical Properties

Property code	Value	Unit	Source
gf	89.43	kJ/mol	Joback Method
hf	-58.70	kJ/mol	Joback Method
hfus	13.90	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.027		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	427.00	K	NIST Webbook
tc	619.39	K	Joback Method
tf	246.44	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.69	J/mol×K	440.98	Joback Method
cpg	228.42	J/mol×K	470.71	Joback Method
cpg	237.72	J/mol×K	500.45	Joback Method
cpg	246.58	J/mol×K	530.18	Joback Method
cpg	255.04	J/mol×K	559.92	Joback Method
cpg	263.10	J/mol×K	589.65	Joback Method
cpg	270.79	J/mol×K	619.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64196e+01
Coeff. B	-4.55664e+03
Coeff. C	-6.71610e+01
Temperature range (K), min.	349.15
Temperature range (K), max.	477.15

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61996790&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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