

1-Hexyn-3-ol

Other names:	1-Hexyne-3-ol 1-Propylpropargyl alcohol 3-Hydroxy-1-hexyne Hexynol Propylethinylcarbinol hex-1-yn-3-ol
Inchi:	InChI=1S/C6H10O/c1-3-5-6(7)4-2/h2,6-7H,3,5H2,1H3
InchiKey:	LTFTWJYRQNTCHI-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	C#CC(O)CCC
Mol. weight [g/mol]:	98.14
CAS:	105-31-7

Physical Properties

Property code	Value	Unit	Source
gf	83.45	kJ/mol	Joback Method
hf	-32.78	kJ/mol	Joback Method
hfus	14.84	kJ/mol	Joback Method
hvap	45.10	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.781		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	415.50 ± 0.50	K	NIST Webbook
tc	594.25	K	Joback Method
tf	250.17	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.65	J/mol×K	418.54	Joback Method
cpg	188.90	J/mol×K	447.83	Joback Method
cpg	196.77	J/mol×K	477.11	Joback Method

cpg	204.30	J/mol×K	506.40	Joback Method
cpg	211.48	J/mol×K	535.68	Joback Method
cpg	218.34	J/mol×K	564.97	Joback Method
cpg	224.88	J/mol×K	594.25	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64587e+01
Coeff. B	-4.24882e+03
Coeff. C	-5.66590e+01
Temperature range (K), min.	319.15
Temperature range (K), max.	438.15

Sources

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=C105317&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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