

3-Hexyn-1-ol

Other names:	3-Hexyne-1-ol 3-Hexynol hex-3-yn-1-ol
Inchi:	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h7H,2,5-6H2,1H3
InchiKey:	ODEHKVYXWLXRRR-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CCC#CCCO
Mol. weight [g/mol]:	98.14
CAS:	1002-28-4

Physical Properties

Property code	Value	Unit	Source
gf	65.62	kJ/mol	Joback Method
hf	-47.10	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	47.78	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.782		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	413.50 ± 0.50	K	NIST Webbook
tc	620.62	K	Joback Method
tf	324.30	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.77	J/mol×K	437.86	Joback Method
cpg	186.99	J/mol×K	468.32	Joback Method
cpg	194.89	J/mol×K	498.78	Joback Method
cpg	202.48	J/mol×K	529.24	Joback Method
cpg	209.77	J/mol×K	559.70	Joback Method
cpg	216.77	J/mol×K	590.16	Joback Method

cpg	223.48	J/mol×K	620.62	Joback Method
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Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	336.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64464e+01
Coeff. B	-4.34111e+03
Coeff. C	-5.98080e+01
Temperature range (K), min.	328.15
Temperature range (K), max.	450.15

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=C1002284&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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