

3-Octyn-1-ol

Other names:	oct-3-yn-1-ol
Inchi:	InChI=1S/C8H14O/c1-2-3-4-5-6-7-8-9/h9H,2-4,7-8H2,1H3
InchiKey:	LRZGRGVRZSDRTK-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CCCCC#CCCO
Mol. weight [g/mol]:	126.20
CAS:	14916-80-4

Physical Properties

Property code	Value	Unit	Source
gf	82.46	kJ/mol	Joback Method
hf	-88.38	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.562		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	483.62	K	Joback Method
tc	663.12	K	Joback Method
tf	346.84	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.31	J/mol×K	483.62	Joback Method
cpg	268.89	J/mol×K	513.54	Joback Method
cpg	279.05	J/mol×K	543.45	Joback Method
cpg	288.79	J/mol×K	573.37	Joback Method
cpg	298.13	J/mol×K	603.29	Joback Method
cpg	307.08	J/mol×K	633.20	Joback Method
cpg	315.65	J/mol×K	663.12	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.00	K	12.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63973e+01
Coeff. B	-4.75406e+03
Coeff. C	-7.38950e+01
Temperature range (K), min.	369.15
Temperature range (K), max.	503.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14916804&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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