

3-Heptyn-1-ol

Other names:	hept-3-yn-1-ol
Inchi:	InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h8H,2-3,6-7H2,1H3
InchiKey:	PSWHODJVUOXHKA-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CCCC#CCCO
Mol. weight [g/mol]:	112.17
CAS:	14916-79-1

Physical Properties

Property code	Value	Unit	Source
gf	74.04	kJ/mol	Joback Method
hf	-67.74	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	50.01	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.172		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	460.74	K	Joback Method
tc	641.90	K	Joback Method
tf	335.57	K	Joback Method
vc	0.408	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.45	J/molxK	460.74	Joback Method
cpg	226.91	J/molxK	490.93	Joback Method
cpg	236.00	J/molxK	521.13	Joback Method
cpg	244.72	J/molxK	551.32	Joback Method
cpg	253.09	J/molxK	581.52	Joback Method
cpg	261.11	J/molxK	611.71	Joback Method
cpg	268.80	J/molxK	641.90	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

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/ci9903071
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=C14916791&Units=SI

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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