3-Hexyn-2-ol

Other names: hex-3-yn-2-ol
Inchi: InChI=1S/C6H10O/c1-3-4-5-6(2)7/h6-7H,3H2,1-2H3
InchiKey: IFCAMPHNVKBSTF-UHFFFAOYSA-N
Formula: C6H10O
SMILES: CCC#CC(C)O
Mol. weight [g/mol]: 98.14
CAS: 109-50-2

Physical Properties

Property code	Value	Unit	Source
gf	63.18	kJ/mol	Joback Method
hf	-52.38	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	47.39	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.781		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
rinpol	796.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	796.00		NIST Webbook
tb	437.42	K	Joback Method
tc	624.36	K	Joback Method
tf	309.30	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.90	J/mol×K	437.42	Joback Method
cpg	187.39	J/mol×K	468.58	Joback Method
cpg	195.55	J/mol×K	499.73	Joback Method
cpg	203.37	J/mol×K	530.89	Joback Method
cpg	210.87	J/mol×K	562.04	Joback Method

cpg	218.05	J/mol×K	593.20	Joback Method
cpg	224.92	J/mol×K	624.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.00	K	8.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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: 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=C109502&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume