5-Hexyn-1-ol

Other names: 1-Hydroxy-5-hexyne
6-Hydroxy-1-hexyne
Hex-5-yn-1-ol
Inchi: InChI=1S/C6H10O/c1-2-3-4-5-6-7/h1,7H,3-6H2
InchiKey: GOQJMMHTSOQIEI-UHFFFAOYSA-N
Formula: C6H10O
SMILES: C#CCCCCO
Mol. weight [g/mol]: 98.14
CAS: 928-90-5

Physical Properties

Property code	Value	Unit	Source
gf	85.89	kJ/mol	Joback Method
hf	-27.50	kJ/mol	Joback Method
hfus	18.36	kJ/mol	Joback Method
hvap	45.49	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.782		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	418.98	K	Joback Method
tc	590.81	K	Joback Method
tf	265.17	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.58	J/mol×K	418.98	Joback Method
cpg	188.56	J/mol×K	447.62	Joback Method
cpg	196.19	J/mol×K	476.26	Joback Method
cpg	203.50	J/mol×K	504.90	Joback Method
cpg	210.48	J/mol×K	533.54	Joback Method
cpg	217.15	J/mol×K	562.18	Joback Method

cpg	223.54	J/mol×K	590.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.20	K	2.00	NIST Webbook
tbrp	348.00	K	2.10	NIST Webbook
tbrp	348.20	K	2.10	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=C928905&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume