

4-Hexen-1-ol

Other names:	4-Hexenol
Inchi:	InChI=1S/C6H12O/c1-2-3-4-5-6-7/h2-3,7H,4-6H2,1H3/b3-2+
InchiKey:	VTIODUHBZHNXFP-NSCUHMNNSA-N
Formula:	C6H12O
SMILES:	CC=CCCCO
Mol. weight [g/mol]:	100.16
CAS:	6126-50-7

Physical Properties

Property code	Value	Unit	Source
gf	-56.96	kJ/mol	Joback Method
hf	-202.18	kJ/mol	Joback Method
hfus	15.59	kJ/mol	Joback Method
hvap	45.59	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.335		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	848.00		NIST Webbook
rinpol	848.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1408.00		NIST Webbook
tb	433.02	K	Joback Method
tc	601.76	K	Joback Method
tf	213.12	K	Joback Method
vc	0.370	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.78	J/mol×K	433.02	Joback Method
cpg	233.69	J/mol×K	573.64	Joback Method
cpg	226.05	J/mol×K	545.51	Joback Method

cpg	218.06	J/mol×K	517.39	Joback Method
cpg	209.69	J/mol×K	489.27	Joback Method
cpg	200.94	J/mol×K	461.14	Joback Method
cpg	240.99	J/mol×K	601.76	Joback Method
dvisc	0.0002006	Paxs	433.02	Joback Method
dvisc	0.0003473	Paxs	396.37	Joback Method
dvisc	0.0006726	Paxs	359.72	Joback Method
dvisc	0.0015133	Paxs	323.07	Joback Method
dvisc	0.0041899	Paxs	286.42	Joback Method
dvisc	0.0156415	Paxs	249.77	Joback Method
dvisc	0.0918576	Paxs	213.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.67821e+01
Coeff. B	-4.43195e+03
Coeff. C	-6.14270e+01
Temperature range (K), min.	330.12
Temperature range (K), max.	447.80

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6126507&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
dvisc:	Dynamic viscosity

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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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