2-Hexen-1-ol

Other names: 2-hexenol
hex-2-en-1-ol
Inchi: InChI=1S/C6H12O/c1-2-3-4-5-6-7/h4-5,7H,2-3,6H2,1H3
InchiKey: ZCHHRLHTBGRGOT-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CCCC=CCO
Mol. weight [g/mol]: 100.16
CAS: 2305-21-7

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	872.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	849.90		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	854.00		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1408.00		NIST Webbook

ripol	1394.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1390.00		NIST Webbook
tb	433.02	K	Joback Method
tc	601.76	K	Joback Method
tf	213.12	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.78	J/mol×K	433.02	Joback Method
cpg	200.94	J/mol×K	461.14	Joback Method
cpg	209.69	J/mol×K	489.27	Joback Method
cpg	218.06	J/mol×K	517.39	Joback Method
cpg	226.05	J/mol×K	545.51	Joback Method
cpg	233.69	J/mol×K	573.64	Joback Method
cpg	240.99	J/mol×K	601.76	Joback Method
dvisc	0.0918576	Pa×s	213.12	Joback Method
dvisc	0.0156415	Pa×s	249.77	Joback Method
dvisc	0.0041899	Pa×s	286.42	Joback Method
dvisc	0.0015133	Pa×s	323.07	Joback Method
dvisc	0.0006726	Pa×s	359.72	Joback Method
dvisc	0.0003473	Pa×s	396.37	Joback Method
dvisc	0.0002006	Pa×s	433.02	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67197e+01

Coeff. B	-4.41089e+03
Coeff. C	-6.12880e+01
Temperature range (K), min.	329.72
Temperature range (K), max.	447.93

Sources

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=C2305217&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

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