1-Hepten-4-ol

Other names: hept-1-en-4-ol
Inchi: InChI=1S/C7H14O/c1-3-5-7(8)6-4-2/h3,7-8H,1,4-6H2,2H3
InchiKey: AQTUHJABKZECGA-UHFFFAOYSA-N
Formula: C7H14O
SMILES: C=CCC(O)CCC
Mol. weight [g/mol]: 114.19
CAS: 3521-91-3

Physical Properties

Property code	Value	Unit	Source
gf	-43.36	kJ/mol	Joback Method
hf	-219.89	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hvap	46.80	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
ripol	1495.00		NIST Webbook
ripol	1585.00		NIST Webbook
tb	447.98	K	Joback Method
tc	614.85	K	Joback Method
tf	212.71	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.57	J/mol×K	447.98	Joback Method
cpg	278.94	J/mol×K	587.04	Joback Method
cpg	270.26	J/mol×K	559.23	Joback Method
cpg	261.19	J/mol×K	531.42	Joback Method
cpg	251.73	J/mol×K	503.60	Joback Method
cpg	241.86	J/mol×K	475.79	Joback Method

cpg	287.25	J/mol×K	614.85	Joback Method
dvisc	0.0002056	Pa×s	447.98	Joback Method
dvisc	0.0003636	Pa×s	408.77	Joback Method
dvisc	0.0007257	Pa×s	369.56	Joback Method
dvisc	0.0017062	Pa×s	330.35	Joback Method
dvisc	0.0050507	Pa×s	291.13	Joback Method
dvisc	0.0209602	Pa×s	251.92	Joback Method
dvisc	0.1469952	Pa×s	212.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37383e+01
Coeff. B	-3.57362e+03
Coeff. C	-6.00370e+01
Temperature range (K), min.	299.15
Temperature range (K), max.	484.11

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3521913&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:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume