4-Hepten-1-ol

Other names: Hept-4-en-1-ol
Inchi: InChI=1S/C7H14O/c1-2-3-4-5-6-7-8/h3-4,8H,2,5-7H2,1H3/b4-3+
InchiKey: CUKAXHVLXKIPKF-ONEGZZNKSA-N
Formula: C7H14O
SMILES: CCC=CCCCO
Mol. weight [g/mol]: 114.19
CAS: 20851-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-48.54	kJ/mol	Joback Method
hf	-222.82	kJ/mol	Joback Method
hfus	18.18	kJ/mol	Joback Method
hvap	47.81	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.725		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	870.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1502.00		NIST Webbook
tb	455.90	K	Joback Method
tc	623.65	K	Joback Method
tf	224.39	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.48	J/mol×K	455.90	Joback Method
cpg	241.71	J/mol×K	483.86	Joback Method
cpg	251.49	J/mol×K	511.82	Joback Method
cpg	260.84	J/mol×K	539.78	Joback Method

cpg	269.79	J/mol×K	567.74	Joback Method
cpg	278.34	J/mol×K	595.69	Joback Method
cpg	286.52	J/mol×K	623.65	Joback Method
dvisc	0.0712349	Pa×s	224.39	Joback Method
dvisc	0.0124675	Pa×s	262.97	Joback Method
dvisc	0.0034085	Pa×s	301.56	Joback Method
dvisc	0.0012506	Pa×s	340.14	Joback Method
dvisc	0.0005629	Pa×s	378.73	Joback Method
dvisc	0.0002936	Pa×s	417.31	Joback Method
dvisc	0.0001710	Pa×s	455.90	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59944e+01
Coeff. B	-4.38019e+03
Coeff. C	-6.68480e+01
Temperature range (K), min.	345.72
Temperature range (K), max.	476.87

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20851552&Units=SI

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