3-Hepten-1-ol

Other names: 3-Heptenol
Inchi: InChI=1S/C7H14O/c1-2-3-4-5-6-7-8/h4-5,8H,2-3,6-7H2,1H3
InchiKey: SDZQUCJFTUULJX-UHFFFAOYSA-N
Formula: C7H14O
SMILES: CCCC=CCCO
Mol. weight [g/mol]: 114.19
CAS: 10606-47-0

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	940.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		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

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=C10606470&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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