3-Hepten-2-ol, (E)-

Other names: (3E)-3-Hepten-2-ol
(E)-3-Hepten-2-ol
trans-3-Hepten-2-ol
Inchi: InChI=1S/C7H14O/c1-3-4-5-6-7(2)8/h5-8H,3-4H2,1-2H3/b6-5+
InchiKey: BOEWENCXVIMZRU-AATRIKPKSA-N
Formula: C7H14O
SMILES: CCCC=CC(C)O
Mol. weight [g/mol]: 114.19
CAS: 67077-39-8

Physical Properties

Property code	Value	Unit	Source
gf	-50.98	kJ/mol	Joback Method
hf	-228.10	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	47.42	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
tb	455.46	K	Joback Method
tc	626.76	K	Joback Method
tf	209.39	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.62	J/mol×K	455.46	Joback Method
cpg	279.70	J/mol×K	598.21	Joback Method
cpg	270.95	J/mol×K	569.66	Joback Method
cpg	261.78	J/mol×K	541.11	Joback Method

cpg	252.19	J/mol×K	512.56	Joback Method
cpg	242.14	J/mol×K	484.01	Joback Method
cpg	288.05	J/mol×K	626.76	Joback Method
dvisc	0.0001634	Pa×s	455.46	Joback Method
dvisc	0.0002941	Pa×s	414.45	Joback Method
dvisc	0.0006019	Pa×s	373.44	Joback Method
dvisc	0.0014702	Pa×s	332.43	Joback Method
dvisc	0.0046173	Pa×s	291.41	Joback Method
dvisc	0.0210963	Pa×s	250.40	Joback Method
dvisc	0.1747804	Pa×s	209.39	Joback Method

Sources

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=C67077398&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
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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