1-Hepten-3-ol

Other names:	Hept-1-en-3-ol
	Heptene-1-ol-3
	NSC 93797
Inchi:	InChI=1S/C7H14O/c1-3-5-6-7(8)4-2/h4,7-8H,2-3,5-6H2,1H3
InchiKey:	PZKFYTOLVRCMOA-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	C=CC(O)CCCC
Mol. weight [g/mol]:	114.19
CAS:	4938-52-7

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
rinpol	867.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	868.00		NIST Webbook

rinpol	865.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1341.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1362.00		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	241.86	J/mol×K	475.79	Joback Method
cpg	251.73	J/mol×K	503.60	Joback Method
cpg	261.19	J/mol×K	531.42	Joback Method
cpg	270.26	J/mol×K	559.23	Joback Method
cpg	278.94	J/mol×K	587.04	Joback Method
cpg	287.25	J/mol×K	614.85	Joback Method
dvisc	0.1469952	Pa×s	212.71	Joback Method
dvisc	0.0209602	Pa×s	251.92	Joback Method
dvisc	0.0050507	Pa×s	291.13	Joback Method
dvisc	0.0017062	Pa×s	330.35	Joback Method
dvisc	0.0007257	Pa×s	369.56	Joback Method
dvisc	0.0003636	Pa×s	408.77	Joback Method
dvisc	0.0002056	Pa×s	447.98	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

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=C4938527&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

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