

6-Hepten-3-ol

Inchi:	InChI=1S/C7H14O/c1-3-5-6-7(8)4-2/h3,7-8H,1,4-6H2,2H3
InchiKey:	XFXWEAWJVWCOBF-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	C=CCCC(O)CC
Mol. weight [g/mol]:	114.19
CAS:	19781-77-2

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
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/molxK	447.98	Joback Method
cpg	241.86	J/molxK	475.79	Joback Method
cpg	251.73	J/molxK	503.60	Joback Method
cpg	261.19	J/molxK	531.42	Joback Method
cpg	270.26	J/molxK	559.23	Joback Method
cpg	278.94	J/molxK	587.04	Joback Method
cpg	287.25	J/molxK	614.85	Joback Method
dvisc	0.1469952	Paxs	212.71	Joback Method
dvisc	0.0209602	Paxs	251.92	Joback Method

dvisc	0.0050507	Paxs	291.13	Joback Method
dvisc	0.0017062	Paxs	330.35	Joback Method
dvisc	0.0007257	Paxs	369.56	Joback Method
dvisc	0.0003636	Paxs	408.77	Joback Method
dvisc	0.0002056	Paxs	447.98	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37811e+01
Coeff. B	-3.59039e+03
Coeff. C	-6.00370e+01
Temperature range (K), min.	326.12
Temperature range (K), max.	483.95

Sources

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=C19781772&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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