

2-Heptenol

Other names:	2-hepten-1-ol
Inchi:	InChI=1S/C7H14O/c1-2-3-4-5-6-7-8/h5-6,8H,2-4,7H2,1H3/b6-5-
InchiKey:	ASFYPVGAALGVNR-WAYWQWQ TSA-N
Formula:	C7H14O
SMILES:	CCCCCC=CCO
Mol. weight [g/mol]:	114.19
CAS:	22104-77-4

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	1052.00		NIST Webbook
rinpol	1051.00		NIST Webbook
ripol	1308.00		NIST Webbook
tb	455.90	K	Joback Method
tc	623.65	K	Joback Method
tf	224.39	K	Joback Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.48	J/mol×K	455.90	Joback Method
cpg	278.34	J/mol×K	595.69	Joback Method
cpg	269.79	J/mol×K	567.74	Joback Method
cpg	260.84	J/mol×K	539.78	Joback Method
cpg	251.49	J/mol×K	511.82	Joback Method

cpg	241.71	J/mol×K	483.86	Joback Method
cpg	286.52	J/mol×K	623.65	Joback Method
dvisc	0.0001710	Paxs	455.90	Joback Method
dvisc	0.0002936	Paxs	417.31	Joback Method
dvisc	0.0005629	Paxs	378.73	Joback Method
dvisc	0.0012506	Paxs	340.14	Joback Method
dvisc	0.0034085	Paxs	301.56	Joback Method
dvisc	0.0124675	Paxs	262.97	Joback Method
dvisc	0.0712349	Paxs	224.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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=C22104774&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

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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