2-Heptenal

Other names: 2-Hepten-1-al
hept-2-enal
Inchi: InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h5-7H,2-4H2,1H3
InchiKey: NDFKTBCGKNOHPJ-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CCCCC=CC=O
Mol. weight [g/mol]: 112.17
CAS: 2463-63-0

Physical Properties

Property code	Value	Unit	Source
gf	-11.24	kJ/mol	Joback Method
hf	-156.17	kJ/mol	Joback Method
hfus	16.38	kJ/mol	Joback Method
hvap	37.85	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	954.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	940.00		NIST Webbook

rinpol	961.00	NIST Webbook
rinpol	975.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	935.00	NIST Webbook
rinpol	940.00	NIST Webbook
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rinpol	945.00	NIST Webbook
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rinpol	909.00	NIST Webbook
rinpol	968.00	NIST Webbook
rinpol	936.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	930.00	NIST Webbook
rinpol	957.00	NIST Webbook
rinpol	951.00	NIST Webbook
rinpol	962.00	NIST Webbook
rinpol	970.00	NIST Webbook
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rinpol	964.00	NIST Webbook
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rinpol	958.00	NIST Webbook
rinpol	963.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1364.00	NIST Webbook
ripol	1353.00	NIST Webbook
ripol	1338.00	NIST Webbook
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ripol	1320.00	NIST Webbook
ripol	1352.00	NIST Webbook
ripol	1337.00	NIST Webbook

ripol	1336.00		NIST Webbook
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ripol	1320.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1321.00		NIST Webbook
tb	412.38	K	Joback Method
tc	592.75	K	Joback Method
tf	205.57	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.75	J/mol×K	412.38	Joback Method
cpg	212.47	J/mol×K	442.44	Joback Method
cpg	222.70	J/mol×K	472.50	Joback Method
cpg	232.44	J/mol×K	502.57	Joback Method
cpg	241.72	J/mol×K	532.63	Joback Method
cpg	250.55	J/mol×K	562.69	Joback Method
cpg	258.96	J/mol×K	592.75	Joback Method
dvisc	0.0042661	Pa×s	205.57	Joback Method
dvisc	0.0019261	Pa×s	240.04	Joback Method
dvisc	0.0010618	Pa×s	274.51	Joback Method
dvisc	0.0006685	Pa×s	308.98	Joback Method
dvisc	0.0004619	Pa×s	343.44	Joback Method
dvisc	0.0003414	Pa×s	377.91	Joback Method
dvisc	0.0002654	Pa×s	412.38	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55564e+01
Coeff. B	-4.04756e+03
Coeff. C	-6.32340e+01
Temperature range (K), min.	328.32
Temperature range (K), max.	458.31

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2463630&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
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

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