

5-heptenal

Inchi:	InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h2-3,7H,4-6H2,1H3/b3-2+
InchiKey:	UDOAKURRCZMWOJ-NSCUHMNNSA-N
Formula:	C7H12O
SMILES:	CC=CCCCCC=O
Mol. weight [g/mol]:	112.17
CAS:	---

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	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
ripol	1276.00		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/molxK	412.38	Joback Method
cpg	212.47	J/molxK	442.44	Joback Method
cpg	222.70	J/molxK	472.50	Joback Method
cpg	232.44	J/molxK	502.57	Joback Method
cpg	241.72	J/molxK	532.63	Joback Method
cpg	250.55	J/molxK	562.69	Joback Method

cpg	258.96	J/mol×K	592.75	Joback Method
dvisc	0.0042661	Paxs	205.57	Joback Method
dvisc	0.0019261	Paxs	240.04	Joback Method
dvisc	0.0010618	Paxs	274.51	Joback Method
dvisc	0.0006685	Paxs	308.98	Joback Method
dvisc	0.0004619	Paxs	343.44	Joback Method
dvisc	0.0003414	Paxs	377.91	Joback Method
dvisc	0.0002654	Paxs	412.38	Joback Method

Correlations

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

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

https://www.chemeo.com/doc/models/crippen_log10ws

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R206581&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

Latest version available from:

<https://www.cheméo.com/cid/69-106-8/5-heptenal.pdf>

Generated by Cheméo on 2024-04-18 19:34:35.253849231 +0000 UTC m=+15758124.174426547.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.