4-Heptenal, (E)-

Other names:	Hept-trans-4-enal
	(E)-4-Heptenal
	(E)-hept-4-enal
Inchi:	InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h3-4,7H,2,5-6H2,1H3/b4-3+
InchiKey:	VVGOCOMZRGWHPI-ONEGZZNKSA-N
Formula:	C7H12O
SMILES:	CCC=CCCC=O
Mol. weight [g/mol]:	112.17
CAS:	929-22-6

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	905.00		NIST Webbook
rinpol	905.00		NIST Webbook
ripol	1234.00		NIST Webbook
ripol	1234.00		NIST Webbook
ripol	1271.00		NIST Webbook
ripol	1234.00		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	250.55	J/mol×K	562.69	Joback Method
cpg	241.72	J/mol×K	532.63	Joback Method
cpg	232.44	J/mol×K	502.57	Joback Method
cpg	222.70	J/mol×K	472.50	Joback Method
cpg	212.47	J/mol×K	442.44	Joback Method
cpg	258.96	J/mol×K	592.75	Joback Method
dvisc	0.0002654	Pa×s	412.38	Joback Method
dvisc	0.0003414	Pa×s	377.91	Joback Method
dvisc	0.0004619	Pa×s	343.44	Joback Method
dvisc	0.0006685	Pa×s	308.98	Joback Method
dvisc	0.0010618	Pa×s	274.51	Joback Method
dvisc	0.0019261	Pa×s	240.04	Joback Method
dvisc	0.0042661	Pa×s	205.57	Joback Method

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=C929226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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