(Z)-4-Heptenal

Other names: 4-heptenal, (Z)-
Inchi: InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h3-4,7H,2,5-6H2,1H3/b4-3-
InchiKey: VVGOCOMZRGWHPI-ARJAWSKDSA-N
Formula: C7H12O
SMILES: CCC=CCCC=O
Mol. weight [g/mol]: 112.17

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	901.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1237.00		NIST Webbook
ripol	1237.00		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

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=R611953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination of Henry s Law Constants and Activity Coefficients at Infinite Dilution of Flavor Compounds in Water at 298 K with a Gas-Chromatographic Method:	https://www.doi.org/10.1021/je0495942

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

Latest version available from:
https://www.chemeo.com/cid/71-711-3/Z-4-Heptenal.pdf
Generated by Cheméo on 2024-04-25 14:00:03.826024066 +0000 UTC m=+16342852.746601383.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.