1-Heptenal

Inchi: InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h6H,2-5H2,1H3
InchiKey: VPGHGGRZCMHQCC-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CCCCCC=C=O
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
gf	-22.00	kJ/mol	Joback Method
hf	-158.22	kJ/mol	Joback Method
hfus	21.42	kJ/mol	Joback Method
hvap	37.35	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	1.955		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	901.00		NIST Webbook
rinpol	901.00		NIST Webbook
tb	353.71	K	Joback Method
tc	516.34	K	Joback Method
tf	191.07	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.04	J/mol×K	353.71	Joback Method
cpg	195.32	J/mol×K	380.81	Joback Method
cpg	205.17	J/mol×K	407.92	Joback Method
cpg	214.60	J/mol×K	435.02	Joback Method
cpg	223.62	J/mol×K	462.13	Joback Method
cpg	232.25	J/mol×K	489.23	Joback Method
cpg	240.51	J/mol×K	516.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522764&Units=SI
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume