4-Ethyl-2-hexynal

Other names: Hex-2-ynal, 4-ethyl-
Inchi: InChI=1S/C8H12O/c1-3-8(4-2)6-5-7-9/h7-8H,3-4H2,1-2H3
InchiKey: XZYAPQCJDYFPBN-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CCC(C#CC=O)CC
Mol. weight [g/mol]: 124.18
CAS: 71932-97-3

Physical Properties

Property code	Value	Unit	Source
gf	117.32	kJ/mol	Joback Method
hf	-27.01	kJ/mol	Joback Method
hfus	18.36	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
ie	10.00	eV	NIST Webbook
log10ws	-2.00		Crippen Method
logp	1.625		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	439.66	K	Joback Method
tc	638.58	K	Joback Method
tf	313.02	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.40	J/mol×K	439.66	Joback Method
cpg	239.81	J/mol×K	472.81	Joback Method
cpg	250.72	J/mol×K	505.97	Joback Method
cpg	261.14	J/mol×K	539.12	Joback Method
cpg	271.08	J/mol×K	572.27	Joback Method
cpg	280.55	J/mol×K	605.42	Joback Method
cpg	289.57	J/mol×K	638.58	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=C71932973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume