2-ethyl-2-hexenal (E)

Other names: (E)-2-Ethylhex-2-enal
Inchi: InChI=1S/C8H14O/c1-3-5-6-8(4-2)7-9/h6-7H,3-5H2,1-2H3/b8-6+
InchiKey: PYLMCYQHBRSDND-SOFGYWHQSA-N
Formula: C8H14O
SMILES: CCCC=C(C=O)CC
Mol. weight [g/mol]: 126.20

Physical Properties

Property code	Value	Unit	Source
gf	-11.37	kJ/mol	Joback Method
hf	-186.60	kJ/mol	Joback Method
hfus	17.66	kJ/mol	Joback Method
hvap	40.16	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1021.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	989.00		NIST Webbook
ripol	1322.00		NIST Webbook
tb	435.14	K	Joback Method
tc	617.65	K	Joback Method
tf	202.88	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.01	J/mol×K	435.14	Joback Method
cpg	253.06	J/mol×K	465.56	Joback Method
cpg	264.55	J/mol×K	495.98	Joback Method
cpg	275.48	J/mol×K	526.39	Joback Method
cpg	285.90	J/mol×K	556.81	Joback Method

cpg	295.81	J/mol×K	587.23	Joback Method
cpg	305.24	J/mol×K	617.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C645625&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume