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

Physical Properties

Property code	Value	Unit	Source
hfus	18.36	kJ/mol	Joback Method
ie	10.00	eV	NIST Webbook
logp	1.625		Crippen Method
mcvol	116.550	ml/mol	McGowan 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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71932973&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume