Pent-2-ynal

Other names: 2-Pentynal
Inchi: InChI=1S/C5H6O/c1-2-3-4-5-6/h5H,2H2,1H3
InchiKey: VLTOSDJJTWPWLS-UHFFFAOYSA-N
Formula: C5H6O
SMILES: CCC#CC=O
Mol. weight [g/mol]: 82.10
CAS: 55136-52-2

Physical Properties

Property code	Value	Unit	Source
gf	94.50	kJ/mol	Joback Method
hf	40.19	kJ/mol	Joback Method
hfus	14.12	kJ/mol	Joback Method
hvap	35.60	kJ/mol	Joback Method
ie	10.12	eV	NIST Webbook
log10ws	-0.99		Crippen Method
logp	0.599		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
ripol	1211.00		NIST Webbook
tb	371.46	K	Joback Method
tc	570.89	K	Joback Method
tf	294.21	K	Joback Method
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.77	J/mol×K	371.46	Joback Method
cpg	127.39	J/mol×K	404.70	Joback Method
cpg	133.75	J/mol×K	437.94	Joback Method
cpg	139.85	J/mol×K	471.17	Joback Method
cpg	145.71	J/mol×K	504.41	Joback Method
cpg	151.31	J/mol×K	537.65	Joback Method

cpg	156.68	J/mol×K	570.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53978e+01
Coeff. B	-3.77345e+03
Coeff. C	-5.23920e+01
Temperature range (K), min.	302.12
Temperature range (K), max.	426.51

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=C55136522&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap:	Vapor pressure

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