2-Butenal, 2-ethyl-

Other names:	2-Ethyl-2-butenal
	2-Ethylcrotonaldehyde
	CH3CH=C(C2H5)CHO
	Crotonaldehyde, 2-ethyl-
Inchi:	InChI=1S/C6H10O/c1-3-6(4-2)5-7/h3,5H,4H2,1-2H3
InchiKey:	IQGZCSXWIRBTRW-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CC=C(C=O)CC
Mol. weight [g/mol]:	98.14
CAS:	19780-25-7

Physical Properties

Property code	Value	Unit	Source
gf	-28.21	kJ/mol	Joback Method
hf	-145.32	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	35.71	kJ/mol	Joback Method
ie	9.53	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	808.00		NIST Webbook
rinpol	793.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1145.00		NIST Webbook
tb	389.38	K	Joback Method
tc	574.52	K	Joback Method
tf	180.34	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	164.68	J/mol×K	389.38	Joback Method
cpg	174.31	J/mol×K	420.24	Joback Method
cpg	183.47	J/mol×K	451.09	Joback Method
cpg	192.18	J/mol×K	481.95	Joback Method
cpg	200.45	J/mol×K	512.80	Joback Method
cpg	208.31	J/mol×K	543.66	Joback Method
cpg	215.78	J/mol×K	574.52	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63924e+01
Coeff. B	-4.10817e+03
Coeff. C	-5.79100e+01
Temperature range (K), min.	313.00
Temperature range (K), max.	428.65

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19780257&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

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

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
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