2-Butenal, 2-ethenyl-

Other names:	Crotonaldehyde, 2-vinyl-
	2-Vinyl-2-butenal
	2-Ethenyl-2-butenal
	2-Vinylcrotonaldehyde
Inchi:	InChI=1S/C6H8O/c1-3-6(4-2)5-7/h3-5H,1H2,2H3/b6-4-
InchiKey:	XOBGIOGZLQNHMM-XQRVVYSFSA-N
Formula:	C6H8O
SMILES:	C=CC(C=O)=CC
Mol. weight [g/mol]:	96.13
CAS:	20521-42-0

Physical Properties

Property code	Value	Unit	Source
gf	59.63	kJ/mol	Joback Method
hf	-19.89	kJ/mol	Joback Method
hfus	11.20	kJ/mol	Joback Method
hvap	35.04	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.318		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	821.00		NIST Webbook
rinpol	821.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1293.00		NIST Webbook
tb	386.06	K	Joback Method
tc	575.25	K	Joback Method
tf	178.58	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.49	J/mol×K	386.06	Joback Method

cpg	159.43	J/mol×K	417.59	Joback Method
cpg	167.87	J/mol×K	449.12	Joback Method
cpg	175.85	J/mol×K	480.66	Joback Method
cpg	183.38	J/mol×K	512.19	Joback Method
cpg	190.48	J/mol×K	543.72	Joback Method
cpg	197.18	J/mol×K	575.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20521420&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
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
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