

2-Butenal, (Z)-

Other names:	(2Z)-2-Butenal (Z)-2-Butenal (Z)-Crotonaldehyde Crotonaldehyde, (Z)- cis-Crotonaldehyde
Inchi:	InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3/b3-2-
InchiKey:	MLUCVPSAIODCQM-IHWYPQMZSA-N
Formula:	C4H6O
SMILES:	CC=CC=O
Mol. weight [g/mol]:	70.09
CAS:	15798-64-8

Physical Properties

Property code	Value	Unit	Source
gf	-36.50	kJ/mol	Joback Method
hf	-94.25	kJ/mol	Joback Method
hfus	8.61	kJ/mol	Joback Method
hvap	31.18	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.761		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
ripol	1035.00		NIST Webbook
tb	343.74	K	Joback Method
tc	526.38	K	Joback Method
tf	171.76	K	Joback Method
vc	0.257	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	97.86	J/molxK	343.74	Joback Method
cpg	127.50	J/molxK	495.94	Joback Method
cpg	122.18	J/molxK	465.50	Joback Method

cpg	116.57	J/molxK	435.06	Joback Method
cpg	110.66	J/molxK	404.62	Joback Method
cpg	104.42	J/molxK	374.18	Joback Method
cpg	132.55	J/molxK	526.38	Joback Method
dvisc	0.0002298	Paxs	343.74	Joback Method
dvisc	0.0002883	Paxs	315.08	Joback Method
dvisc	0.0003783	Paxs	286.41	Joback Method
dvisc	0.0005275	Paxs	257.75	Joback Method
dvisc	0.0007992	Paxs	229.09	Joback Method
dvisc	0.0013638	Paxs	200.42	Joback Method
dvisc	0.0027814	Paxs	171.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46487e+01
Coeff. B	-3.32715e+03
Coeff. C	-4.54420e+01
Temperature range (K), min.	277.12
Temperature range (K), max.	401.77

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15798648&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/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity

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

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