2-Butenal, (E)-

Other names:	(E)-2-Butenal
	(E)-But-2-enal
	(E)-Crotonaldehyde
	2-Butenal, (2E)-
	Aldehyde crotonique
	But-(E)-2-enal
	Crotonal
	Crotonaldehyde
	Crotonaldehyde, (E)-
	E-Crotonic aldehyde
	E-Crotylaldehyde
	NCI-C56279
	Rcra waste number U053
	Topanel
	Topanel CA
	t-2-Butenal
	trans-2-Butenal
	trans-Crotonal
	trans-Crotonaldehyde
	«beta»-Methyl acrolein, trans
	Â«betaÂ»-Methyl acrolein, trans
Inchi:	InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3/b3-2+
InchiKey:	MLUCVPSAIODCQM-NSCUHMNNSA-N
Formula:	C4H6O
SMILES:	CC=CC=O
Mol. weight [g/mol]:	70.09
CAS:	123-73-9

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
ie	9.73	eV	NIST Webbook
log10ws	-0.63		Crippen Method

logp	0.761		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
rinpol	648.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	648.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	645.00		NIST Webbook
rinpol	624.00		NIST Webbook
rinpol	619.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1023.00		NIST Webbook
ripol	1084.00		NIST Webbook
ripol	1050.00		NIST Webbook
ripol	1038.00		NIST Webbook
ripol	1035.00		NIST Webbook
ripol	1044.00		NIST Webbook
ripol	1050.00		NIST Webbook
ripol	1002.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1040.00		NIST Webbook
ripol	1046.00		NIST Webbook
ripol	1034.00		NIST Webbook
ripol	1044.00		NIST Webbook
ripol	1047.00		NIST Webbook
ripol	1043.00		NIST Webbook
ripol	1036.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1035.00		NIST Webbook
ripol	1033.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1032.00		NIST Webbook
ripol	1012.00		NIST Webbook

ripol	1034.00		NIST Webbook
ripol	1043.00		NIST Webbook
tb	375.35	K	NIST Webbook
tb	375.15 ± 2.00	K	NIST Webbook
tb	377.70	K	NIST Webbook
tc	526.38	K	Joback Method
tf	196.55 ± 0.20	K	NIST Webbook
tf	198.15	K	NIST Webbook
vc	0.257	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.55	J/mol×K	526.38	Joback Method
cpg	122.18	J/mol×K	465.50	Joback Method
cpg	127.50	J/mol×K	495.94	Joback Method
cpg	97.86	J/mol×K	343.74	Joback Method
cpg	104.42	J/mol×K	374.18	Joback Method
cpg	110.66	J/mol×K	404.62	Joback Method
cpg	116.57	J/mol×K	435.06	Joback Method
cpl	148.60	J/mol×K	298.35	NIST Webbook
cpl	148.60	J/mol×K	298.35	NIST Webbook
dvisc	0.0002298	Pa×s	343.74	Joback Method
dvisc	0.0003783	Pa×s	286.41	Joback Method
dvisc	0.0002883	Pa×s	315.08	Joback Method
dvisc	0.0027814	Pa×s	171.76	Joback Method
dvisc	0.0013638	Pa×s	200.42	Joback Method
dvisc	0.0007992	Pa×s	229.09	Joback Method
dvisc	0.0005275	Pa×s	257.75	Joback Method
hvapt	32.10 ± 0.50	kJ/mol	362.50	NIST Webbook
hvapt	34.50 ± 0.20	kJ/mol	362.50	NIST Webbook
hvapt	36.60 ± 0.10	kJ/mol	362.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.45589e+01
Coeff. B	-3.30226e+03
Coeff. C	-4.54980e+01
Temperature range (K), min.	276.89
Temperature range (K), max.	402.60

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123739&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
Measurement of activity coefficient at infinite dilution for some bio-oil components in water and mass transfer	https://www.doi.org/10.1016/j.fluid.2015.01.010
Solubility of carbon monoxides in bio-oil compounds:	https://www.doi.org/10.1016/j.jct.2016.10.030
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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