2-Butenal, 2-methyl-, (E)-

Other names:	(2E)-2-Methyl-2-butenal
	(E)-2-Methylbut-2-enal
	2-Butenal, 2-methyl-, (2E)-
	2-Methyl-(E)-2-butenal
	2-Methyl-2(E)-butenal
	2-Methyl-2-butenal, (E)
	2-Methyl-2-butenal, trans
	2-Methylbut-(E)-2-enal
	Crotonaldehyde, 2-methyl-, (E)-
	E-2-Methyl-2-butenal
	NSC 2179
	Tiglaldehyde
	Tiglaldehyde (2-Methyl-2-butenal)
	Tiglic acid aldehyde
	Tiglic aldehyde
	trans-2-Methyl-2-butenal
	trans-Tiglaldehyde
Inchi:	InChI=1S/C5H8O/c1-3-5(2)4-6/h3-4H,1-2H3/b5-3-
InchiKey:	ACWQBUSCFPJUPN-HYXAFXHYSA-N
Formula:	C5H8O
SMILES:	CC=C(C)C=O
Mol. weight [g/mol]:	84.12
CAS:	497-03-0

Physical Properties

Property code	Value	Unit	Source
chl	-2879.00	kJ/mol	NIST Webbook
gf	-36.63	kJ/mol	Joback Method
hf	-124.68	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	33.48	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	763.00		NIST Webbook

rinpol	737.00	NIST Webbook
rinpol	745.00	NIST Webbook
rinpol	724.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	745.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	738.00	NIST Webbook
rinpol	745.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	738.00	NIST Webbook
ripol	1069.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1084.00	NIST Webbook
ripol	1092.00	NIST Webbook
ripol	1090.00	NIST Webbook
ripol	1082.00	NIST Webbook
ripol	1094.00	NIST Webbook
ripol	1092.00	NIST Webbook
ripol	1082.00	NIST Webbook
ripol	1084.00	NIST Webbook
ripol	1082.00	NIST Webbook
ripol	1097.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1098.00	NIST Webbook
ripol	1076.00	NIST Webbook
ripol	1091.00	NIST Webbook
ripol	1094.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1098.00	NIST Webbook
ripol	1075.00	NIST Webbook
ripol	1074.00	NIST Webbook
ripol	1088.00	NIST Webbook
ripol	1097.00	NIST Webbook
ripol	1101.00	NIST Webbook
ripol	1096.00	NIST Webbook
ripol	1096.00	NIST Webbook
ripol	1113.00	NIST Webbook
ripol	1069.00	NIST Webbook
ripol	1113.00	NIST Webbook
ripol	1113.00	NIST Webbook
ripol	1107.00	NIST Webbook
ripol	1082.00	NIST Webbook

ripol	1098.00		NIST Webbook
ripol	1076.00		NIST Webbook
ripol	1082.00		NIST Webbook
tb	366.50	K	Joback Method
tc	552.54	K	Joback Method
tf	169.07	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.19	J/mol×K	521.53	Joback Method
cpg	130.05	J/mol×K	366.50	Joback Method
cpg	138.26	J/mol×K	397.51	Joback Method
cpg	146.07	J/mol×K	428.51	Joback Method
cpg	153.48	J/mol×K	459.52	Joback Method
cpg	160.51	J/mol×K	490.53	Joback Method
cpg	173.52	J/mol×K	552.54	Joback Method
hvapt	39.20	kJ/mol	319.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.70	K	100.00	NIST Webbook
tbrp	337.20	K	15.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48810e+01
Coeff. B	-3.49905e+03
Coeff. C	-4.97510e+01
Temperature range (K), min.	289.52

Temperature range (K), max.	415.40

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C497030&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume