2-Butenal, 2-methyl-

Other names:	2,3-Dimethylacrolein
	2-Methyl-2-butenal
	2-Methylbut-2-enal
	2-Methylcrotonaldehyde
	Crotonaldehyde, 2-methyl-
Inchi:	InChI=1S/C5H8O/c1-3-5(2)4-6/h3-4H,1-2H3
InchiKey:	ACWQBUSCFPJUPN-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	CC=C(C)C=O
Mol. weight [g/mol]:	84.12
CAS:	1115-11-3

Physical Properties

Property code	Value	Unit	Source
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
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	715.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	730.00		NIST Webbook

rinpol	737.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	741.00	NIST Webbook
ripol	1100.00	NIST Webbook
ripol	1095.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1063.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1088.00	NIST Webbook
ripol	1095.00	NIST Webbook
ripol	1095.00	NIST Webbook
ripol	1109.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1119.00	NIST Webbook
ripol	1085.00	NIST Webbook
ripol	1104.00	NIST Webbook
ripol	1084.00	NIST Webbook
ripol	1108.00	NIST Webbook
ripol	1073.00	NIST Webbook
ripol	1102.00	NIST Webbook
ripol	1102.00	NIST Webbook
ripol	1102.00	NIST Webbook
ripol	1114.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1073.00	NIST Webbook
ripol	1129.00	NIST Webbook
ripol	1091.00	NIST Webbook
ripol	1090.00	NIST Webbook
ripol	1101.00	NIST Webbook
ripol	1101.00	NIST Webbook
ripol	1101.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1087.00	NIST Webbook
ripol	1097.00	NIST Webbook
ripol	1093.00	NIST Webbook
ripol	1129.00	NIST Webbook
ripol	1101.00	NIST Webbook
ripol	1097.00	NIST Webbook
ripol	1076.00	NIST Webbook
ripol	1090.00	NIST Webbook
ripol	1101.00	NIST Webbook
ripol	1100.00	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	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	167.19	J/mol×K	521.53	Joback Method
cpg	173.52	J/mol×K	552.54	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64097e+01
Coeff. B	-3.86560e+03
Coeff. C	-4.97510e+01
Temperature range (K), min.	289.52
Temperature range (K), max.	398.06

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1115113&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
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