2-BUTENAL, 3-METHYL-

Other names:	3,3-Dimethylacrolein
	3-Methyl-2-butenal
	3-Methyl-2-butenaldehyde
	3-Methylbut-2-enal
	3-Methylcrotonaldehyde
	3-methyl-2-butenal (prenal)
	Crotonaldehyde, 3-methyl-
	NSC 149164
	Prenal
	Senecialdehyde
	Senecioaldehyde
	«beta»,«beta»-Dimethylacrolein
	«beta»,«beta»-Dimethylacrylic aldehyde
	«beta»-Methylcrotonaldehyde
Inchi:	InChI=1S/C5H8O/c1-5(2)3-4-6/h3-4H,1-2H3
InchiKey:	SEPQTYODOKLVSB-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	CC(C)=CC=O
Mol. weight [g/mol]:	84.12
CAS:	107-86-8

Physical Properties

Property code	Value	Unit	Source
affp	856.90	kJ/mol	NIST Webbook
basg	825.00	kJ/mol	NIST Webbook
hf	-143.99	kJ/mol	Cheméo Relay (1.0)
hfus	9.89	kJ/mol	Joback Method
hvap	39.83	kJ/mol	Cheméo Relay (1.0)
ie	9.25	eV	Cheméo Relay (1.0)
log10ws	-0.24		Cheméo Relay (1.0)
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
rinpol	753.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	780.00		NIST Webbook

rinpol	748.40	NIST Webbook
rinpol	784.00	NIST Webbook
rinpol	787.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	755.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	781.00	NIST Webbook
rinpol	748.40	NIST Webbook
rinpol	783.30	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	800.00	NIST Webbook
rinpol	796.00	NIST Webbook
rinpol	758.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	753.00	NIST Webbook
rinpol	744.00	NIST Webbook
ripol	1189.00	NIST Webbook
ripol	1236.00	NIST Webbook
ripol	1222.00	NIST Webbook
ripol	1215.00	NIST Webbook
ripol	1212.00	NIST Webbook
ripol	1220.50	NIST Webbook
ripol	1189.00	NIST Webbook
ripol	1215.00	NIST Webbook
ripol	1221.00	NIST Webbook
ripol	1199.00	NIST Webbook
ripol	1202.00	NIST Webbook
ripol	1230.00	NIST Webbook
ripol	1200.00	NIST Webbook
ripol	1220.50	NIST Webbook
ripol	1215.00	NIST Webbook
ripol	1202.00	NIST Webbook

ripol	1236.00		NIST Webbook
ripol	1206.00		NIST Webbook
ripol	1233.00		NIST Webbook
ripol	1199.00		NIST Webbook
tb	407.20	K	NIST Webbook
tf	249.69	K	Cheméo Relay (1.0)

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	1.49139e+01
Coeff. B	-3.63291e+03
Coeff. C	-5.43380e+01
Temperature range (K), min.	302.72
Temperature range (K), max.	432.67

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107868&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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