2-Pentenal, 2-methyl-

Other names:	2-Methyl-2-penten-1-al
	2-Methyl-2-pentenal
	2-Methyl-2-pentene-1-al
	2-Methyl-2-pentenoic aldehyde
	2-Methyl-3-ethylacrolein
	2-Methylpent-2-enal
	CH3CH2CH=C(CH3)CHO
	NSC 9464
	«alpha»-Methyl-«beta»-ethylacrolein
	«beta»-Ethyl-«alpha»-methylacrolein
	Â«alphaÂ»-Methyl-Â«betaÂ»-ethylacrolein
	Â«betaÂ»-Ethyl-Â«alphaÂ»-methylacrolein
Inchi:	InChI=1S/C6H10O/c1-3-4-6(2)5-7/h4-5H,3H2,1-2H3
InchiKey:	IDEYZABHVQLHAF-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CCC=C(C)C=O
Mol. weight [g/mol]:	98.14
CAS:	623-36-9

Physical Properties

Property code	Value	Unit	Source
chl	-3783.00	kJ/mol	NIST Webbook
gf	-28.21	kJ/mol	Joback Method
hf	-145.32	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	35.71	kJ/mol	Joback Method
ie	9.54	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	808.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	850.00		NIST Webbook

rinpol	808.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	829.70		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	829.70		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	809.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	828.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1157.00		NIST Webbook
ripol	1155.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1172.00		NIST Webbook
ripol	1157.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1155.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1155.00		NIST Webbook
ripol	1155.00		NIST Webbook
ripol	1151.00		NIST Webbook
tb	409.15 ± 2.00	K	NIST Webbook
tc	574.52	K	Joback Method

tf	178.60 ± 0.60	K	NIST Webbook
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.68	J/mol×K	389.38	Joback Method
cpg	174.31	J/mol×K	420.24	Joback Method
cpg	183.47	J/mol×K	451.09	Joback Method
cpg	192.18	J/mol×K	481.95	Joback Method
cpg	200.45	J/mol×K	512.80	Joback Method
cpg	208.31	J/mol×K	543.66	Joback Method
cpg	215.78	J/mol×K	574.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.70	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50236e+01
Coeff. B	-3.68324e+03
Coeff. C	-5.51720e+01
Temperature range (K), min.	305.12
Temperature range (K), max.	434.41

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623369&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

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
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