Methacrolein

Other names:	.alpha.-methylacrolein
	2-Methylacrolein
	2-Methylenepropanal
	2-Methylprop-2-enal
	2-Propenal, 2-methyl-
	2-methyl-2-propenal
	2-methylpropenal
	Acrolein, 2-methyl-
	CH2=C(CH3)CHO
	Isobutenal
	Methacraldehyde
	Methacrylic aldehyde
	Methakrylaldehyd
	Methylacroleine
	Methylacrylaldehyde
	NSC 8260
	methacrylaldehyde
	«alpha»-Methacrolein
	«alpha»-Methylacrolein
Inchi:	InChI=1S/C4H6O/c1-4(2)3-5/h3H,1H2,2H3
InchiKey:	STNJBCKSHOAVAJ-UHFFFAOYSA-N
Formula:	C4H6O
SMILES:	C=C(C)C=O
Mol. weight [g/mol]:	70.09
CAS:	78-85-3

Physical Properties

Property code	Value	Unit	Source
affp	808.70	kJ/mol	NIST Webbook
basg	776.80	kJ/mol	NIST Webbook
chl	-2293.00 ± 1.90	kJ/mol	NIST Webbook
gf	-37.43	kJ/mol	Joback Method
hf	-106.40 ± 2.00	kJ/mol	NIST Webbook
hfl	-138.60 ± 2.00	kJ/mol	NIST Webbook
hfus	5.82	kJ/mol	Joback Method
hvap	32.20	kJ/mol	NIST Webbook
ie	9.92	eV	NIST Webbook

log10ws	-0.63		Crippen Method
logp	0.761		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
rinpol	556.00		NIST Webbook
rinpol	552.70		NIST Webbook
rinpol	574.00		NIST Webbook
rinpol	577.00		NIST Webbook
rinpol	566.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	552.00		NIST Webbook
rinpol	531.00		NIST Webbook
rinpol	568.40		NIST Webbook
rinpol	543.00		NIST Webbook
ripol	893.00		NIST Webbook
ripol	885.00		NIST Webbook
ripol	883.00		NIST Webbook
ripol	891.00		NIST Webbook
ripol	884.00		NIST Webbook
tb	342.15	K	NIST Webbook
tb	341.60	K	NIST Webbook
tc	516.54	K	Joback Method
tf	192.15	K	NIST Webbook
vc	0.259	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	99.74	J/mol×K	336.14	Joback Method
cpg	106.03	J/mol×K	366.21	Joback Method
cpg	112.04	J/mol×K	396.27	Joback Method
cpg	117.78	J/mol×K	426.34	Joback Method
cpg	123.26	J/mol×K	456.41	Joback Method
cpg	128.49	J/mol×K	486.48	Joback Method
cpg	133.48	J/mol×K	516.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and predicted excess molar enthalpies of binary mixtures containing 2,2′-oxybis[propane], benzene, butan-1-ol, 2-methylpropan-1-ol, and 2-methylprop-2-en-1-ol:	https://www.doi.org/10.1016/j.fluid.2010.08.024
Phase Equilibrium Measurements of the Methacrolein+Methacrylic Acid+Water Ternary System at 101.3 kPa:	https://www.doi.org/10.1021/acs.jced.9b00649
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=C78853&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hfl:	Liquid phase 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
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