

2-Butenoic acid, 2-methyl-, (Z)-

Other names:	(2Z)-2-Methyl-2-butenoic acid (Z) CH ₃ CH=C(CH ₃)COOH (Z)-2-Methyl-2-butenoic acid 2-Methyl-2-butenoic acid, cis 2-methylisocrotonic acid Angelic acid Crotonic acid, 2-methyl-, (Z)- cis-2-Methyl-2-butenoic acid
Inchi:	InChI=1S/C5H8O2/c1-3-4(2)5(6)7/h3H,1-2H3,(H,6,7)/b4-3-
InchiKey:	UIERETOOQGIECD-ARJAWSKDSA-N
Formula:	C ₅ H ₈ O ₂
SMILES:	CC=C(C)C(=O)O
Mol. weight [g/mol]:	100.12
CAS:	565-63-9

Physical Properties

Property code	Value	Unit	Source
affp	822.50	kJ/mol	NIST Webbook
basg	791.50	kJ/mol	NIST Webbook
gf	-202.85	kJ/mol	Joback Method
hf	-303.91	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	50.19	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	1.037		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4491.67 ± 100.00	kPa	NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	919.70		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1849.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1779.00		NIST Webbook
ripol	1849.00		NIST Webbook
tb	458.20	K	NIST Webbook
tc	661.14 ± 3.00	K	NIST Webbook
tf	237.82	K	Joback Method

vc

0.322

m³/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.96	J/mol×K	617.27	Joback Method
cpg	166.62	J/mol×K	463.89	Joback Method
cpg	174.00	J/mol×K	494.57	Joback Method
cpg	181.01	J/mol×K	525.24	Joback Method
cpg	187.67	J/mol×K	555.92	Joback Method
cpg	193.97	J/mol×K	586.60	Joback Method
cpg	205.63	J/mol×K	647.95	Joback Method
hvapt	61.80	kJ/mol	409.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.26996e+01
Coeff. B	-2.62487e+03
Coeff. C	-1.42737e+02
Temperature range (K), min.	354.22
Temperature range (K), max.	498.02

Sources

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=C565639&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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

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