

2-Propenoic acid, 2-methyl-, 1-methylethyl ester

Other names:	1-methylethyl 2-methyl-2-propenoate Acrylic acid, 2-methyl-, isopropyl ester Isopropyl 2-methyl-2-propenoate Isopropyl methacrylate Methacrylic acid isopropyl ester
Inchi:	InChI=1S/C7H12O2/c1-5(2)7(8)9-6(3)4/h6H,1H2,2-4H3
InchiKey:	BOQSSGDQNWFSX-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=C(C)C(=O)OC(C)C
Mol. weight [g/mol]:	128.17
CAS:	4655-34-9

Physical Properties

Property code	Value	Unit	Source
gf	-149.01	kJ/mol	Joback Method
hf	-322.25	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	39.35	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.514		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	811.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	807.00		NIST Webbook
ripol	1039.00		NIST Webbook
ripol	1043.00		NIST Webbook
tb	431.97	K	Joback Method
tc	619.68	K	Joback Method
tf	210.09	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.88	J/mol×K	431.97	Joback Method
cpg	233.85	J/mol×K	463.25	Joback Method
cpg	244.40	J/mol×K	494.54	Joback Method
cpg	254.52	J/mol×K	525.82	Joback Method
cpg	264.23	J/mol×K	557.11	Joback Method
cpg	273.52	J/mol×K	588.39	Joback Method
cpg	282.41	J/mol×K	619.68	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34337e+01
Coeff. B	-3.25213e+03
Coeff. C	-5.18360e+01
Temperature range (K), min.	299.22
Temperature range (K), max.	452.24

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Phase behavior measurement on the
binary mixture for isopropyl acrylate
and isobutyl methacrylate in

<https://www.doi.org/10.1016/j.fluid.2006.08.019>

supercritical CO₂:
McGowan Method:

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

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4655349&Units=SI>

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

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