

Propanoic acid, 2-methyl-, 2-propenyl ester

Other names:	Isobutyric acid, allyl ester allyl isobutyrate
Inchi:	InChI=1S/C7H12O2/c1-4-5-9-7(8)6(2)3/h4,6H,1,5H2,2-3H3
InchiKey:	QNBDJTKBKITRJI-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	C=CCOC(=O)C(C)C
Mol. weight [g/mol]:	128.17
CAS:	15727-77-2

Physical Properties

Property code	Value	Unit	Source
gf	-140.46	kJ/mol	Joback Method
hf	-312.46	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	39.27	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.372		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	815.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	815.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1090.00		NIST Webbook
tb	432.09	K	Joback Method
tc	616.21	K	Joback Method
tf	224.05	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.93	J/mol×K	432.09	Joback Method

cpg	272.85	J/mol×K	585.52	Joback Method
cpg	263.67	J/mol×K	554.84	Joback Method
cpg	254.10	J/mol×K	524.15	Joback Method
cpg	244.12	J/mol×K	493.46	Joback Method
cpg	233.73	J/mol×K	462.78	Joback Method
cpg	281.64	J/mol×K	616.21	Joback Method
dvisc	0.0002529	Pa×s	432.09	Joback Method
dvisc	0.0003294	Pa×s	397.42	Joback Method
dvisc	0.0004515	Pa×s	362.74	Joback Method
dvisc	0.0006615	Pa×s	328.07	Joback Method
dvisc	0.0010605	Pa×s	293.40	Joback Method
dvisc	0.0019297	Pa×s	258.72	Joback Method
dvisc	0.0042260	Pa×s	224.05	Joback Method

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=C15727772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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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