Allyl isovalerate

Other names:	2-Propenyl 3-methylbutanoate
	2-Propenyl isovalerate
	3-Methylbutanoic acid, 2-propenyl ester
	3-Methylbutyric acid, allyl ester
	Allyl 3-methylbutyrate
	Allyl isopentanoate
	Allyl isovalerianate
	Butanoic acid, 3-methyl-, 2-propen-1-yl ester
	Butanoic acid, 3-methyl-, 2-propenyl ester
	Butyric acid, 3-methyl-, allyl ester
	FEMA No. 2045
	Isovaleric acid, allyl ester
	NCI-C54717
	NSC 18606
Inchi:	InChI=1S/C8H14O2/c1-4-5-10-8(9)6-7(2)3/h4,7H,1,5-6H2,2-3H3
InchiKey:	HOMAGVUCNZNWBC-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	C=CCOC(=O)CC(C)C
Mol. weight [g/mol]:	142.20
CAS:	2835-39-4

Physical Properties

Property code	Value	Unit	Source
gf	-132.04	kJ/mol	Joback Method
hf	-333.10	kJ/mol	Joback Method
hfus	14.46	kJ/mol	Joback Method
hvap	41.50	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.762		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	920.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	915.00		NIST Webbook
ripol	1190.00		NIST Webbook

ripol	1190.00		NIST Webbook
tb	454.97	K	Joback Method
tc	637.48	K	Joback Method
tf	235.32	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.19	J/mol×K	454.97	Joback Method
cpg	318.44	J/mol×K	607.06	Joback Method
cpg	308.30	J/mol×K	576.64	Joback Method
cpg	297.72	J/mol×K	546.22	Joback Method
cpg	286.67	J/mol×K	515.81	Joback Method
cpg	275.17	J/mol×K	485.39	Joback Method
cpg	328.12	J/mol×K	637.48	Joback Method
dvisc	0.0002428	Pa×s	454.97	Joback Method
dvisc	0.0003181	Pa×s	418.36	Joback Method
dvisc	0.0004389	Pa×s	381.75	Joback Method
dvisc	0.0006484	Pa×s	345.14	Joback Method
dvisc	0.0010509	Pa×s	308.54	Joback Method
dvisc	0.0019397	Pa×s	271.93	Joback Method
dvisc	0.0043324	Pa×s	235.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57003e+01
Coeff. B	-4.73278e+03
Coeff. C	-8.29300e+01
Temperature range (K), min.	390.00
Temperature range (K), max.	538.49

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=C2835394&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

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
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