

2-Butenoic acid, 2-methyl-, 2-propenyl ester, (E)-

Other names:	Tiglic acid, allyl ester Allyl tiglate Allyl trans-2-methyl-2-butenate allyl 2-methylcrotonate
Inchi:	InChI=1S/C8H12O2/c1-4-6-10-8(9)7(3)5-2/h4-5H,1,6H2,2-3H3/b7-5+
InchiKey:	ODOZNBUSHKFCSH-FNORWQNLSA-N
Formula:	C8H12O2
SMILES:	C=CCOC(=O)C(C)=CC
Mol. weight [g/mol]:	140.18
CAS:	7493-71-2

Physical Properties

Property code	Value	Unit	Source
gf	-57.93	kJ/mol	Joback Method
hf	-220.39	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	41.93	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.682		Crippen Method
mcvol	122.420	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	1021.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1002.00		NIST Webbook
ripol	1370.00		NIST Webbook
tb	459.45	K	Joback Method
tc	650.12	K	Joback Method
tf	231.28	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.55	J/molxK	459.45	Joback Method

cpg	257.99	J/mol×K	491.23	Joback Method
cpg	268.90	J/mol×K	523.01	Joback Method
cpg	279.29	J/mol×K	554.79	Joback Method
cpg	289.18	J/mol×K	586.56	Joback Method
cpg	298.60	J/mol×K	618.34	Joback Method
cpg	307.55	J/mol×K	650.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C7493712&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
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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