

2-Butenoic acid, 2-propenyl ester

Other names:	Crotonic acid, allyl ester Allyl crotonate Allyl (2e)-2-butenate allyl 2-butenate
Inchi:	InChI=1S/C7H10O2/c1-3-5-7(8)9-6-4-2/h3-5H,2,6H2,1H3/b5-3+
InchiKey:	WNJBUWVXSNLWEQ-HWKANZROSA-N
Formula:	C7H10O2
SMILES:	<chem>C=CCOC(=O)C=CC</chem>
Mol. weight [g/mol]:	126.15
CAS:	20474-93-5

Physical Properties

Property code	Value	Unit	Source
gf	-57.80	kJ/mol	Joback Method
hf	-189.96	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	39.62	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.292		Crippen Method
mcvol	108.330	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	436.69	K	Joback Method
tc	625.64	K	Joback Method
tf	233.97	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.84	J/molxK	436.69	Joback Method
cpg	216.93	J/molxK	468.18	Joback Method
cpg	226.56	J/molxK	499.67	Joback Method
cpg	235.74	J/molxK	531.17	Joback Method
cpg	244.49	J/molxK	562.66	Joback Method

cpg	252.82	J/molxK	594.15	Joback Method
cpg	260.75	J/molxK	625.64	Joback Method
dvisc	0.0026175	Paxs	233.97	Joback Method
dvisc	0.0013346	Paxs	267.76	Joback Method
dvisc	0.0007914	Paxs	301.54	Joback Method
dvisc	0.0005214	Paxs	335.33	Joback Method
dvisc	0.0003708	Paxs	369.12	Joback Method
dvisc	0.0002792	Paxs	402.90	Joback Method
dvisc	0.0002196	Paxs	436.69	Joback Method

Sources

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=C20474935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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