

Propanoic acid, 2-propenyl ester

Other names:	Propionic acid, allyl ester Allyl propionate <chem>C2H5C(O)OCH2CH=CH2</chem> Allyl n-propionate
Inchi:	InChI=1S/C6H10O2/c1-3-5-8-6(7)4-2/h3H,1,4-5H2,2H3
InchiKey:	XRFWKHVQMACVTA-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	<chem>C=CCOC(=O)CC</chem>
Mol. weight [g/mol]:	114.14
CAS:	2408-20-0

Physical Properties

Property code	Value	Unit	Source
gf	-146.44	kJ/mol	Joback Method
hf	-286.54	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	37.44	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	776.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	738.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1128.00		NIST Webbook

ripol	1130.00		NIST Webbook
ripol	1130.00		NIST Webbook
tb	409.65	K	Joback Method
tc	590.97	K	Joback Method
tf	227.78	K	Joback Method
vc	0.377	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.90	J/mol×K	409.65	Joback Method
cpg	194.08	J/mol×K	439.87	Joback Method
cpg	202.94	J/mol×K	470.09	Joback Method
cpg	211.47	J/mol×K	500.31	Joback Method
cpg	219.68	J/mol×K	530.53	Joback Method
cpg	227.57	J/mol×K	560.75	Joback Method
cpg	235.15	J/mol×K	590.97	Joback Method
dvisc	0.0026729	Pa×s	227.78	Joback Method
dvisc	0.0014557	Pa×s	258.09	Joback Method
dvisc	0.0009008	Pa×s	288.40	Joback Method
dvisc	0.0006108	Pa×s	318.72	Joback Method
dvisc	0.0004430	Pa×s	349.03	Joback Method
dvisc	0.0003382	Pa×s	379.34	Joback Method
dvisc	0.0002688	Pa×s	409.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2408200&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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