Allyl propionate

Other names:	Propionic acid, allyl ester
	Allyl propionate
	C2H5C(O)OCH2CH=CH2
	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:	C=CCOC(=O)CC
Mol. weight [g/mol]:	114.14

Physical Properties

Property code	Value	Unit	Source
af	0.3837		Cheméo Relay (1.0)
gf	-146.44	kJ/mol	Joback Method
hf	-350.40	kJ/mol	Cheméo Relay (1.0)
hfus	12.80	kJ/mol	Joback Method
hvap	39.75	kJ/mol	Cheméo Relay (1.0)
ie	9.75	eV	Cheméo Relay (1.0)
log10ws	-0.82		Cheméo Relay (1.0)
logp	1.126		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	818.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	796.00		NIST Webbook
ripol	1130.00		NIST Webbook

ripol	1128.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1130.00		NIST Webbook
tb	395.08	K	Cheméo Relay (1.0)
tc	575.34	K	Cheméo Relay (1.0)
tf	181.20	K	Cheméo Relay (1.0)
vc	0.353	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2408200&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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