Allyl 2-ethyl butyrate

Other names:	Butanoic acid, 2-ethyl-, 2-propenyl ester
	Butyric acid, 2-ethyl-, allyl ester
	2-Propenyl 2-ethylbutanoate
	Allyl 2-ethylbutanoate
Inchi:	InChI=1S/C9H16O2/c1-4-7-11-9(10)8(5-2)6-3/h4,8H,1,5-7H2,2-3H3
InchiKey:	NBKXNUWCFMZFMM-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	C=CCOC(=O)C(CC)CC
Mol. weight [g/mol]:	156.22
CAS:	7493-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-123.62	kJ/mol	Joback Method
hf	-353.74	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	43.73	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	995.00		NIST Webbook
ripol	1254.00		NIST Webbook
tb	477.85	K	Joback Method
tc	658.67	K	Joback Method
tf	246.59	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.61	J/mol×K	477.85	Joback Method
cpg	318.63	J/mol×K	507.99	Joback Method
cpg	331.13	J/mol×K	538.12	Joback Method

cpg	343.12	J/mol×K	568.26	Joback Method
cpg	354.60	J/mol×K	598.39	Joback Method
cpg	365.59	J/mol×K	628.53	Joback Method
cpg	376.08	J/mol×K	658.67	Joback Method
dvisc	0.0043503	Pa×s	246.59	Joback Method
dvisc	0.0019129	Pa×s	285.13	Joback Method
dvisc	0.0010229	Pa×s	323.68	Joback Method
dvisc	0.0006250	Pa×s	362.22	Joback Method
dvisc	0.0004198	Pa×s	400.76	Joback Method
dvisc	0.0003024	Pa×s	439.31	Joback Method
dvisc	0.0002296	Pa×s	477.85	Joback Method

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=C7493698&Units=SI
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
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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