Decanoic acid, 2-propenyl ester

Other names:	Allyl caprate
	Allyl n-decanoate
	Allyl decanoate
Inchi:	InChI=1S/C13H24O2/c1-3-5-6-7-8-9-10-11-13(14)15-12-4-2/h4H,2-3,5-12H2,1H3
InchiKey:	DQVOTEHORLHPRW-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	C=CCOC(=O)CCCCCCCCC
Mol. weight [g/mol]:	212.33
CAS:	57856-81-2

Physical Properties

Property code	Value	Unit	Source
gf	-87.50	kJ/mol	Joback Method
hf	-431.02	kJ/mol	Joback Method
hfus	30.93	kJ/mol	Joback Method
hvap	53.02	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.856		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1476.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1458.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1752.00		NIST Webbook
tb	569.81	K	Joback Method
tc	741.25	K	Joback Method
tf	306.67	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.21	J/mol×K	569.81	Joback Method
cpg	566.84	J/mol×K	712.68	Joback Method
cpg	553.58	J/mol×K	684.10	Joback Method
cpg	539.69	J/mol×K	655.53	Joback Method
cpg	525.18	J/mol×K	626.96	Joback Method
cpg	510.03	J/mol×K	598.38	Joback Method
cpg	579.50	J/mol×K	741.25	Joback Method
dvisc	0.0001759	Pa×s	569.81	Joback Method
dvisc	0.0002301	Pa×s	525.95	Joback Method
dvisc	0.0003162	Pa×s	482.10	Joback Method
dvisc	0.0004631	Pa×s	438.24	Joback Method
dvisc	0.0007382	Pa×s	394.38	Joback Method
dvisc	0.0013224	Pa×s	350.53	Joback Method
dvisc	0.0027987	Pa×s	306.67	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57856812&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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