Octanoic acid, 2-propenyl ester

Other names:	Allyl caprylate
	Allyl n-octanoate
	Allyl octanoate
	Octanoic acid, allyl ester
Inchi:	InChI=1S/C11H20O2/c1-3-5-6-7-8-9-11(12)13-10-4-2/h4H,2-3,5-10H2,1H3
InchiKey:	PZGMUSDNQDCNAG-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	C=CCOC(=O)CCCCCCC
Mol. weight [g/mol]:	184.28
CAS:	4230-97-1

Physical Properties

Property code	Value	Unit	Source
gf	-104.34	kJ/mol	Joback Method
hf	-389.74	kJ/mol	Joback Method
hfus	25.75	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1265.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1265.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1554.00		NIST Webbook
tb	524.05	K	Joback Method
tc	698.08	K	Joback Method
tf	284.13	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.19	J/mol×K	524.05	Joback Method
cpg	410.62	J/mol×K	553.05	Joback Method
cpg	424.47	J/mol×K	582.06	Joback Method
cpg	437.74	J/mol×K	611.06	Joback Method
cpg	450.46	J/mol×K	640.07	Joback Method
cpg	462.62	J/mol×K	669.07	Joback Method
cpg	474.25	J/mol×K	698.08	Joback Method
dvisc	0.0029982	Pa×s	284.13	Joback Method
dvisc	0.0014650	Pa×s	324.12	Joback Method
dvisc	0.0008378	Pa×s	364.10	Joback Method
dvisc	0.0005351	Pa×s	404.09	Joback Method
dvisc	0.0003706	Pa×s	444.08	Joback Method
dvisc	0.0002727	Pa×s	484.06	Joback Method
dvisc	0.0002102	Pa×s	524.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52377e+01
Coeff. B	-4.47881e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	379.22
Temperature range (K), max.	530.85

Sources

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4230971&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor 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