

Hexanoic acid, allyl ester

Other names:	2-Propenyl n-hexanoate 2-propenyl hexanoate Allyl caproate Allyl n-hexanoate Allylester kyseliny kapronove allyl capronate allyl hexanoate
Inchi:	InChI=1S/C9H16O2/c1-3-5-6-7-9(10)11-8-4-2/h4H,2-3,5-8H2,1H3
InchiKey:	RCSBILYQLVXLJG-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	C=CCOC(=O)CCCCC
Mol. weight [g/mol]:	156.23
CAS:	123-68-2

Physical Properties

Property code	Value	Unit	Source
af	0.5224		Cheméo Relay (1.0)
hf	-429.88	kJ/mol	Cheméo Relay (1.0)
hfus	20.57	kJ/mol	Joback Method
hvap	49.83	kJ/mol	Cheméo Relay (1.0)
ie	9.70	eV	Cheméo Relay (1.0)
log10ws	-2.50		Cheméo Relay (1.0)
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1062.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1056.00		NIST Webbook

ripol	1061.00		NIST Webbook
ripol	1080.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1370.00		NIST Webbook
tb	452.37	K	Cheméo Relay (1.0)
tc	639.03	K	Cheméo Relay (1.0)
tf	197.25	K	Cheméo Relay (1.0)
vc	0.512	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.44	J/mol×K	478.29	Joback Method
cpg	374.26	J/mol×K	655.34	Joback Method
cpg	363.97	J/mol×K	625.83	Joback Method
cpg	353.22	J/mol×K	596.32	Joback Method
cpg	342.00	J/mol×K	566.81	Joback Method
cpg	330.31	J/mol×K	537.31	Joback Method
cpg	318.12	J/mol×K	507.80	Joback Method
dvisc	0.0005918	Pa×s	369.94	Joback Method
dvisc	0.0002419	Pa×s	478.29	Joback Method
dvisc	0.0003104	Pa×s	442.17	Joback Method
dvisc	0.0004165	Pa×s	406.06	Joback Method
dvisc	0.0030378	Pa×s	261.59	Joback Method
dvisc	0.0009072	Pa×s	333.82	Joback Method
dvisc	0.0015428	Pa×s	297.71	Joback Method
hvapt	55.20	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50787e+01
Coeff. B	-4.13006e+03
Coeff. C	-6.87940e+01
Temperature range (K), min.	348.02
Temperature range (K), max.	491.64

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C123682&Units=SI>

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

Cheméo Relay (1.0, beta):

Vapor pressures and vaporization enthalpies of a series of esters used in <https://www.doi.org/10.1016/j.jct.2015.02.015>

The Yaws Handbook of Vapor Pressure <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure Enthalpy: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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

Crippen Method:

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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

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