

allyl 3,5,5-trimethylhexanoate

Inchi:	InChI=1S/C12H22O2/c1-6-7-14-11(13)8-10(2)9-12(3,4)5/h6,10H,1,7-9H2,2-5H3
InchiKey:	NSXNWIWVNIJLHK-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	C=CCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	198.31
CAS:	71500-21-5

Physical Properties

Property code	Value	Unit	Source
hfus	17.41	kJ/mol	Joback Method
ie	9.50	eV	Cheméo Relay (1.0)
logp	3.178		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
tb	470.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.59	J/mol×K	543.26	Joback Method
cpg	534.60	J/mol×K	728.86	Joback Method
cpg	521.96	J/mol×K	697.93	Joback Method
cpg	508.61	J/mol×K	666.99	Joback Method
cpg	494.53	J/mol×K	636.06	Joback Method
cpg	479.68	J/mol×K	605.13	Joback Method
cpg	464.05	J/mol×K	574.19	Joback Method
dvisc	0.0005458	Pa×s	413.04	Joback Method
dvisc	0.0001688	Pa×s	543.26	Joback Method
dvisc	0.0002333	Pa×s	499.85	Joback Method
dvisc	0.0003427	Pa×s	456.45	Joback Method
dvisc	0.0051988	Pa×s	282.82	Joback Method
dvisc	0.0009699	Pa×s	369.63	Joback Method
dvisc	0.0020082	Pa×s	326.23	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46081e+01
Coeff. B	-4.35803e+03
Coeff. C	-8.25320e+01
Temperature range (K), min.	386.85
Temperature range (K), max.	551.31

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/109-852-5/allyl-3-5-5-trimethylhexanoate.pdf>

Generated by Cheméo on 2026-07-21 23:33:03.439339452 +0000 UTC m=+187879.281224858.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.