

Allyl nonadecanoate

Inchi:	InChI=1S/C22H42O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22(23)24-21-4-2
InchiKey:	LHDOSLHSHKWMXST-UHFFFAOYSA-N
Formula:	C22H42O2
SMILES:	C=CCOC(=O)CCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	338.57

Physical Properties

Property code	Value	Unit	Source
gf	-11.72	kJ/mol	Joback Method
hf	-616.78	kJ/mol	Joback Method
hfus	54.24	kJ/mol	Joback Method
hvap	73.05	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.367		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	951.42	kPa	Joback Method
rinpol	2351.00		NIST Webbook
tb	775.73	K	Joback Method
tc	952.53	K	Joback Method
tf	408.10	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.44	J/molxK	775.73	Joback Method
cpg	1094.96	J/molxK	923.07	Joback Method
cpg	1078.72	J/molxK	893.60	Joback Method
cpg	1061.58	J/molxK	864.13	Joback Method
cpg	1043.51	J/molxK	834.66	Joback Method
cpg	1024.48	J/molxK	805.20	Joback Method
cpg	1110.33	J/molxK	952.53	Joback Method
dvisc	0.0000592	Paxs	775.73	Joback Method
dvisc	0.0000797	Paxs	714.46	Joback Method

dvisc	0.0001134	Paxs	653.19	Joback Method
dvisc	0.0001736	Paxs	591.91	Joback Method
dvisc	0.0002930	Paxs	530.64	Joback Method
dvisc	0.0005673	Paxs	469.37	Joback Method
dvisc	0.0013391	Paxs	408.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541141&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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