

Allyl myristate

Inchi:	InChI=1S/C17H32O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-17(18)19-16-4-2/h4H,2-3,5-16H
InchiKey:	FFXFQWSEFSLIKK-UHFFFAOYSA-N
Formula:	C17H32O2
SMILES:	C=CCOC(=O)CCCCCCCCCCCCC
Mol. weight [g/mol]:	268.43
CAS:	45236-96-2

Physical Properties

Property code	Value	Unit	Source
gf	-53.82	kJ/mol	Joback Method
hf	-513.58	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	61.92	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.417		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	1852.00		NIST Webbook
rinpol	1852.00		NIST Webbook
tb	661.33	K	Joback Method
tc	830.65	K	Joback Method
tf	351.75	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.83	J/mol×K	661.33	Joback Method
cpg	726.69	J/mol×K	689.55	Joback Method
cpg	743.76	J/mol×K	717.77	Joback Method
cpg	760.05	J/mol×K	745.99	Joback Method
cpg	775.61	J/mol×K	774.21	Joback Method
cpg	790.43	J/mol×K	802.43	Joback Method
cpg	804.54	J/mol×K	830.65	Joback Method

dvisc	0.0021607	Pa×s	351.75	Joback Method
dvisc	0.0009658	Pa×s	403.35	Joback Method
dvisc	0.0005182	Pa×s	454.94	Joback Method
dvisc	0.0003156	Pa×s	506.54	Joback Method
dvisc	0.0002107	Pa×s	558.14	Joback Method
dvisc	0.0001506	Pa×s	609.73	Joback Method
dvisc	0.0001135	Pa×s	661.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C45236962&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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