

Valeric acid, undec-2-enyl ester

Inchi:	InChI=1S/C16H30O2/c1-3-5-7-8-9-10-11-12-13-15-18-16(17)14-6-4-2/h12-13H,3-11,14-1
InchiKey:	DNXKABMLNDEGAE-OUKQBFOZSA-N
Formula:	C16H30O2
SMILES:	CCCCCCCCC=CCOC(=O)CCCC
Mol. weight [g/mol]:	254.41

Physical Properties

Property code	Value	Unit	Source
gf	-69.86	kJ/mol	Joback Method
hf	-501.15	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	60.32	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.027		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	1782.00		NIST Webbook
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tb	645.93	K	Joback Method
tc	818.34	K	Joback Method
tf	337.16	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.12	J/mol×K	645.93	Joback Method
cpg	672.59	J/mol×K	674.67	Joback Method
cpg	689.29	J/mol×K	703.40	Joback Method
cpg	705.23	J/mol×K	732.14	Joback Method
cpg	720.44	J/mol×K	760.87	Joback Method
cpg	734.94	J/mol×K	789.61	Joback Method
cpg	748.76	J/mol×K	818.34	Joback Method
dvisc	0.0022449	Pa×s	337.16	Joback Method

dvisc	0.0009605	Pa×s	388.62	Joback Method
dvisc	0.0005012	Pa×s	440.08	Joback Method
dvisc	0.0002997	Pa×s	491.55	Joback Method
dvisc	0.0001976	Pa×s	543.01	Joback Method
dvisc	0.0001400	Pa×s	594.47	Joback Method
dvisc	0.0001048	Pa×s	645.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292491&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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