

Pentanoic acid, 9-decenyl ester

Other names:	9-Decen-1-yl pentanoate
Inchi:	InChI=1S/C15H28O2/c1-3-5-7-8-9-10-11-12-14-17-15(16)13-6-4-2/h3H,1,4-14H2,2H3
InchiKey:	CZQAUYHFZOOTSH-UHFFFAOYSA-N
Formula:	C15H28O2
SMILES:	C=CCCCCCCCCOC(=O)CCCC
Mol. weight [g/mol]:	240.38

Physical Properties

Property code	Value	Unit	Source
gf	-70.66	kJ/mol	Joback Method
hf	-472.30	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.636		Crippen Method
mvol	225.350	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	615.57	K	Joback Method
tc	785.30	K	Joback Method
tf	329.21	K	Joback Method
vc	0.880	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.68	J/mol×K	615.57	Joback Method
cpg	676.23	J/mol×K	757.01	Joback Method
cpg	662.10	J/mol×K	728.72	Joback Method
cpg	647.30	J/mol×K	700.44	Joback Method
cpg	631.81	J/mol×K	672.15	Joback Method
cpg	615.61	J/mol×K	643.86	Joback Method
cpg	689.70	J/mol×K	785.30	Joback Method

dvisc	0.0001429	Paxs	615.57	Joback Method
dvisc	0.0001884	Paxs	567.84	Joback Method
dvisc	0.0002614	Paxs	520.12	Joback Method
dvisc	0.0003874	Paxs	472.39	Joback Method
dvisc	0.0006273	Paxs	424.66	Joback Method
dvisc	0.0011478	Paxs	376.94	Joback Method
dvisc	0.0025018	Paxs	329.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U159933&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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