

4-Pentenoic acid, 2-methyl-, nonyl ester

Inchi:	InChI=1S/C15H28O2/c1-4-6-7-8-9-10-11-13-17-15(16)14(3)12-5-2/h5,14H,2,4,6-13H2,1,
InchiKey:	SUIJFENYPSLILQ-UHFFFAOYSA-N
Formula:	C15H28O2
SMILES:	C=CCC(C)C(=O)OCCCCCCCCC
Mol. weight [g/mol]:	240.38

Physical Properties

Property code	Value	Unit	Source
gf	-73.10	kJ/mol	Joback Method
hf	-477.58	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	57.08	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.492		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	615.13	K	Joback Method
tc	787.46	K	Joback Method
tf	314.21	K	Joback Method
vc	0.875	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.05	J/molxK	615.13	Joback Method
cpg	677.81	J/molxK	758.74	Joback Method
cpg	663.50	J/molxK	730.01	Joback Method
cpg	648.48	J/molxK	701.29	Joback Method
cpg	632.74	J/molxK	672.57	Joback Method
cpg	616.27	J/molxK	643.85	Joback Method
cpg	691.45	J/molxK	787.46	Joback Method
dvisc	0.0001332	Paxs	615.13	Joback Method

dvisc	0.0001794	Paxs	564.98	Joback Method
dvisc	0.0002561	Paxs	514.82	Joback Method
dvisc	0.0003947	Paxs	464.67	Joback Method
dvisc	0.0006755	Paxs	414.52	Joback Method
dvisc	0.0013405	Paxs	364.36	Joback Method
dvisc	0.0033107	Paxs	314.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406112&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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