

2-nonenoic acid «gamma»-lactone

Other names:	5-pentyl-2(5H)-furanone (5H)-5-Pentyl-2-furanone 5-pentylfuran-2(5H)-one
Inchi:	InChI=1S/C9H14O2/c1-2-3-4-5-8-6-7-9(10)11-8/h6-8H,2-5H2,1H3
InchiKey:	MXZSZHJBUODOJK-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CCCCC1C=CC(=O)O1
Mol. weight [g/mol]:	154.21
CAS:	21963-26-8

Physical Properties

Property code	Value	Unit	Source
gf	-117.30	kJ/mol	Joback Method
hf	-380.53	kJ/mol	Joback Method
hfus	21.71	kJ/mol	Joback Method
hvap	44.93	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.048		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1299.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1345.00		NIST Webbook
ripol	2052.00		NIST Webbook
ripol	2068.00		NIST Webbook
ripol	2076.00		NIST Webbook
ripol	2072.00		NIST Webbook
tb	514.53	K	Joback Method
tc	724.15	K	Joback Method
tf	297.64	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.49	J/mol×K	514.53	Joback Method
cpg	320.70	J/mol×K	549.47	Joback Method
cpg	335.19	J/mol×K	584.40	Joback Method
cpg	348.96	J/mol×K	619.34	Joback Method
cpg	362.03	J/mol×K	654.28	Joback Method
cpg	374.41	J/mol×K	689.21	Joback Method
cpg	386.08	J/mol×K	724.15	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21963268&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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