

2-(Nonyloxy)ethanol, acetate

Other names:	2-Nonyloxyethyl acetate
Inchi:	InChI=1S/C13H26O3/c1-3-4-5-6-7-8-9-10-15-11-12-16-13(2)14/h3-12H2,1-2H3
InchiKey:	NFVICYCNBIGUMI-UHFFFAOYSA-N
Formula:	C13H26O3
SMILES:	CCCCCCCCCOCCOC(C)=O
Mol. weight [g/mol]:	230.34

Physical Properties

Property code	Value	Unit	Source
gf	-280.34	kJ/mol	Joback Method
hf	-688.67	kJ/mol	Joback Method
hfus	33.40	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.317		Crippen Method
mvol	207.340	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	1615.50		NIST Webbook
rinpol	1615.50		NIST Webbook
tb	595.55	K	Joback Method
tc	764.22	K	Joback Method
tf	330.66	K	Joback Method
vc	0.805	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.50	J/mol×K	595.55	Joback Method
cpg	559.59	J/mol×K	623.66	Joback Method
cpg	575.06	J/mol×K	651.77	Joback Method
cpg	589.90	J/mol×K	679.89	Joback Method
cpg	604.13	J/mol×K	708.00	Joback Method
cpg	617.73	J/mol×K	736.11	Joback Method
cpg	630.73	J/mol×K	764.22	Joback Method

dvisc	0.0020526	Paxs	330.66	Joback Method
dvisc	0.0009978	Paxs	374.81	Joback Method
dvisc	0.0005647	Paxs	418.96	Joback Method
dvisc	0.0003562	Paxs	463.10	Joback Method
dvisc	0.0002435	Paxs	507.25	Joback Method
dvisc	0.0001769	Paxs	551.40	Joback Method
dvisc	0.0001347	Paxs	595.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184486&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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