

3-Nonyl nitrate

Inchi:	InChI=1S/C9H19NO3/c1-3-5-6-7-8-9(4-2)13-10(11)12/h9H,3-8H2,1-2H3
InchiKey:	YXUXBXICIGKFLH-UHFFFAOYSA-N
Formula:	C9H19NO3
SMILES:	CCCCCCC(CC)O[N+](=O)[O-]
Mol. weight [g/mol]:	189.25

Physical Properties

Property code	Value	Unit	Source
gf	-46.99	kJ/mol	Joback Method
hf	-377.35	kJ/mol	Joback Method
hfus	28.09	kJ/mol	Joback Method
hvap	54.24	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	2.944		Crippen Method
mcvol	160.960	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinsol	1233.00		NIST Webbook
tb	579.14	K	Joback Method
tc	775.17	K	Joback Method
tf	342.03	K	Joback Method
vc	0.633	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.13	J/mol×K	579.14	Joback Method
cpg	425.68	J/mol×K	611.81	Joback Method
cpg	439.54	J/mol×K	644.48	Joback Method
cpg	452.71	J/mol×K	677.16	Joback Method
cpg	465.22	J/mol×K	709.83	Joback Method
cpg	477.07	J/mol×K	742.50	Joback Method
cpg	488.27	J/mol×K	775.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496947&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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