

# 4-Octyl nitrate

<b>Inchi:</b>	InChI=1S/C8H17NO3/c1-3-5-7-8(6-4-2)12-9(10)11/h8H,3-7H2,1-2H3
<b>InchiKey:</b>	KXDZDQGNGXHCGI-UHFFFAOYSA-N
<b>Formula:</b>	C8H17NO3
<b>SMILES:</b>	CCCCC(CCC)O[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	175.23

## Physical Properties

Property code	Value	Unit	Source
gf	-55.41	kJ/mol	Joback Method
hf	-356.71	kJ/mol	Joback Method
hfus	25.50	kJ/mol	Joback Method
hvap	52.02	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.554		Crippen Method
mcvol	146.870	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1122.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1122.00		NIST Webbook
tb	556.26	K	Joback Method
tc	754.99	K	Joback Method
tf	330.76	K	Joback Method
vc	0.578	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.36	J/molxK	556.26	Joback Method
cpg	377.14	J/molxK	589.38	Joback Method
cpg	390.27	J/molxK	622.50	Joback Method
cpg	402.76	J/molxK	655.63	Joback Method
cpg	414.62	J/molxK	688.75	Joback Method
cpg	425.87	J/molxK	721.87	Joback Method
cpg	436.50	J/molxK	754.99	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R496625&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R496625&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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