

Nitric acid, octyl ester

Other names:	1-Octyl nitrate Octyl nitrate n-Octyl nitrate
Inchi:	InChI=1S/C8H17NO3/c1-2-3-4-5-6-7-8-12-9(10)11/h2-8H2,1H3
InchiKey:	TXQBMQNFXYOIPT-UHFFFAOYSA-N
Formula:	C8H17NO3
SMILES:	CCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	175.23
CAS:	629-39-0

Physical Properties

Property code	Value	Unit	Source
gf	-52.97	kJ/mol	Joback Method
hf	-351.43	kJ/mol	Joback Method
hfus	29.03	kJ/mol	Joback Method
hvap	52.40	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.555		Crippen Method
mcvol	146.870	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
tb	556.70	K	Joback Method
tc	751.43	K	Joback Method
tf	345.76	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.01	J/molxK	556.70	Joback Method
cpg	376.46	J/molxK	589.16	Joback Method
cpg	389.28	J/molxK	621.61	Joback Method
cpg	401.51	J/molxK	654.07	Joback Method

cpg	413.13	J/mol×K	686.52	Joback Method
cpg	424.17	J/mol×K	718.98	Joback Method
cpg	434.64	J/mol×K	751.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.33370e+01
Coeff. B	-3.64327e+03
Coeff. C	-7.18100e+01
Temperature range (K), min.	351.00
Temperature range (K), max.	525.77

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629390&Units=SI

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

pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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