

Nitric acid, 1-methylpropyl ester

Other names:	2-Butyl nitrate C2H5CH(CH3)ONO2 Nitric acid, sec-butyl ester sec-Butyl Nitrate
Inchi:	InChI=1S/C4H9NO3/c1-3-4(2)8-5(6)7/h4H,3H2,1-2H3
InchiKey:	DYONNFFVDNILGI-UHFFFAOYSA-N
Formula:	C4H9NO3
SMILES:	CCC(C)O[N+](=O)[O-]
Mol. weight [g/mol]:	119.12
CAS:	924-52-7

Physical Properties

Property code	Value	Unit	Source
gf	-89.09	kJ/mol	Joback Method
hf	-274.15	kJ/mol	Joback Method
hfus	15.14	kJ/mol	Joback Method
hvap	43.11	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	0.993		Crippen Method
mcvol	90.510	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
rinpol	739.00		NIST Webbook
rinpol	739.00		NIST Webbook
tb	397.15 ± 2.00	K	NIST Webbook
tc	675.22	K	Joback Method
tf	285.68	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.08	J/mol×K	464.74	Joback Method
cpg	200.48	J/mol×K	499.82	Joback Method
cpg	209.47	J/mol×K	534.90	Joback Method

cpg	218.07	J/mol×K	569.98	Joback Method
cpg	226.27	J/mol×K	605.06	Joback Method
cpg	234.06	J/mol×K	640.14	Joback Method
cpg	241.46	J/mol×K	675.22	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48992e+01
Coeff. B	-3.55299e+03
Coeff. C	-5.15580e+01
Temperature range (K), min.	294.72
Temperature range (K), max.	422.13

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C924527&Units=SI
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/ci990307l
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
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
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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