

Nitric acid, pentyl ester

Other names:	Amyl nitrate Amylester kyseliny dusicne Nitrate D'amyle Pentyl nitrate UN 1112 n-Amyl nitrate
Inchi:	InChI=1S/C5H11NO3/c1-2-3-4-5-9-6(7)8/h2-5H2,1H3
InchiKey:	HSNWZBCBUUSSQD-UHFFFAOYSA-N
Formula:	C5H11NO3
SMILES:	CCCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	133.15
CAS:	1002-16-0

Physical Properties

Property code	Value	Unit	Source
gf	-78.23	kJ/mol	Joback Method
hf	-289.51	kJ/mol	Joback Method
hfus	21.25	kJ/mol	Joback Method
hvap	45.73	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.385		Crippen Method
mcvol	104.600	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	905.00		NIST Webbook
rinpol	900.00		NIST Webbook
ripol	1220.00		NIST Webbook
tb	488.06	K	Joback Method
tc	690.93	K	Joback Method
tf	311.95	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	230.86	J/mol×K	488.06	Joback Method
cpg	241.26	J/mol×K	521.87	Joback Method
cpg	251.21	J/mol×K	555.68	Joback Method
cpg	260.71	J/mol×K	589.49	Joback Method
cpg	269.78	J/mol×K	623.31	Joback Method
cpg	278.41	J/mol×K	657.12	Joback Method
cpg	286.61	J/mol×K	690.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45226e+01
Coeff. B	-3.66206e+03
Coeff. C	-5.90640e+01
Temperature range (K), min.	316.32
Temperature range (K), max.	456.63

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback 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=C1002160&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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