

Amyl nitrite

Other names:	n-Pentyl nitrite n-Amyl nitrite Nitrous acid, pentyl ester Nitramyl Pentyl alcohol, nitrite Pentyl nitrite
Inchi:	InChI=1S/C5H11NO2/c1-2-3-4-5-8-6-7/h2-5H2,1H3
InchiKey:	CSDTZUBPSYWZDX-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	CCCCCON=O
Mol. weight [g/mol]:	117.15
CAS:	463-04-7

Physical Properties

Property code	Value	Unit	Source
hf	-446.94	kJ/mol	Joback Method
hvap	38.23	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.875		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	695.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	695.00		NIST Webbook
tb	377.70	K	NIST Webbook
tc	567.82	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C463047&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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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