Isoamyl nitrite

Other names:	Nitrous acid, 3-methylbutyl ester
	Isopentyl alcohol, nitrite
	Aspiral
	Isopentyl nitrite
	Nitramyl
	Vaporole
	3-Methylbutanol nitrite
	3-Methylbutyl nitrite
	Amilnitrite
	Nitrous acid, isopentyl ester
	NCI-C50179
	IPN
	NSC 7903
	"amyl nitrite", mixed isomers
	Amyl Nitrite
Inchi:	InChI=1S/C5H11NO2/c1-5(2)3-4-8-6-7/h5H,3-4H2,1-2H3
InchiKey:	OWFXIOWLTKNBAP-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	CC(C)CCON=O
Mol. weight [g/mol]:	117.15
CAS:	110-46-3

Physical Properties

Property code	Value	Unit	Source
hf	-452.22	kJ/mol	Joback Method
hvap	37.84	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.731		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	684.00		NIST Webbook
rinpol	680.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	653.00		NIST Webbook
rinpol	653.00		NIST Webbook
rinpol	684.00		NIST Webbook
tb	372.40	K	NIST Webbook

tb	369.00 ± 1.00	K	NIST Webbook
tc	571.22	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110463&Units=SI
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

hf:	Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature